Four-Dimensional Atmospheric Variational Data Assimilation at NRL

by

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Outline

- Background
- Formulation and implementation
  - A generalized cost function
  - Solution to the Euler-Lagrange system
  - Implementation of NAVDAS-AR
- Data assimilation experiments
  - Initial tests of the inner loop
  - Experiments with the outer loop
  - Preliminary results with SSM/I wind speeds and TPW
- Issues and opportunities
- Concluding remarks

Background

- **NAVDAS:**
  - **NRL Atmospheric Variational Data Assimilation System (Daley and Barker, 2000, 2001). It is a 3DVAR system cast in observation-space.**
- **Representer Algorithm:**
  - **The representer algorithm was introduced into oceanography by Bennett and McIntosh (1982), Bennett and Thorburn (1992). This algorithm is one way to solve the generalized inverse problem – that is, to variationally minimize a generalized four dimensional cost function. The computational cost is proportional to the number of observations.**
- **Accelerated Representer Algorithm:**
  - **A practical way (sub-optimal) to implement the representer algorithm in a cycling operational environment (Xu and Daley, 2002). It is similar to the iterative method described by Egbert et al. (1997), Amodei (1995), Courtier (1998), where it is referred as the 4D-PSAS, and Chua and Bennett (2001).**

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Background …

- **NAVDAS-AR:**
  - **NAVDAS-AR is a natural four dimensional extension of NAVDAS, where "AR" stands for accelerated representer.**
  - **NAVDAS-AR is designed to be used for both the global and regional data assimilation applications.**
  - **However, currently we only apply it to the global application for two reasons: (1) There is no lateral boundary condition in the global case. (2) We have in-house expertise (Tom Rosmond) in the global (NOGAPS) adjoint system.**
  - **NAVDAS-AR uses the existing NAVDAS and NOGAPS (Hogan and Rosmond, 1991) infrastructures. It parallels the 4DVAR algorithm implemented at ECMWF, but is an observation space algorithm, as is NAVDAS, and doesn't require a perfect model assumption.**

Formulation of NAVDAS-AR

A genereralized cost function

$$J = J_0^b + J^q + J^r$$

$$\begin{cases} J_0^b = \frac{1}{2}\left[\mathbf{x}_0^b - \mathbf{x}_0\right]^T \left[\mathbf{P}_0^b\right]^{-1} \left[\mathbf{x}_0^b - \mathbf{x}_0\right], \\ J^q = \frac{1}{2}\sum_{n=1}^{N}\sum_{n'=1}^{N}\left[\mathbf{x}_n - \mathcal{M}\left(\mathbf{x}_{n-1}\right)\right]^T \mathbf{Q}_{nn'}^{-1}\left[\mathbf{x}_{n'} - \mathcal{M}\left(\mathbf{x}_{n'-1}\right)\right], \\ J^r = \frac{1}{2}\left[\mathbf{y} - \mathcal{H}(\mathbf{x})\right]^T \mathbf{R}^{-1}\left[\mathbf{y} - \mathcal{H}(\mathbf{x})\right], \end{cases}$$

where $\mathbf{x}_n^b = \mathcal{M}\left(\mathbf{x}_{n-1}^b\right)$, and $\mathbf{x}_n$ is a state vector at time $\mathbf{t}_n$ of length I. $\mathbf{y}$ is a vector of all observations of length K. $\mathcal{M}$ is a nonlinear prediction model, such as NOGAPS or COAMPS™, $\mathcal{H}$ represents forward (or observation) operators and can be nonlinear. The analysis $\mathbf{x}^a$ is found when $J = J_{min}$. Notice that $\mathbf{P}_0^b$, $\mathbf{Q}_{nn'}$, and $\mathbf{R}$ are error covariances of initial background, model, and observations & (observation operators), respectively.

Formulation of NAVDAS-AR

Two special cost functions

1. 3DVAR:

$$2J_{\min} = \left[\mathbf{x}_0^b - \mathbf{x}_0^a\right]^T \left[\mathbf{P}_0^b\right]^{-1} \left[\mathbf{x}_0^b - \mathbf{x}_0^a\right] + \left[\mathbf{y} - \mathcal{H}(\mathbf{x}_0^a)\right]^T \mathbf{R}^{-1} \left[\mathbf{y} - \mathcal{H}(\mathbf{x}_0^a)\right]$$

Since there is no time evolution, there is no need for a prediction model in the cost function.

There are usually specified simple multivariate relationships, such as the geostrophic relationship (strong or weak constraint).

2. Strong constraint 4DVAR:

$$2J_{\min} = \left[\mathbf{x}_0^b - \mathbf{x}_0^a\right]^T \left[\mathbf{P}_0^b\right]^{-1} \left[\mathbf{x}_0^b - \mathbf{x}_0^a\right] + \left[\mathbf{y} - \mathcal{H}(\mathbf{x}^a)\right]^T \mathbf{R}^{-1} \left[\mathbf{y} - \mathcal{H}(\mathbf{x}^a)\right],$$

$\mathbf{x}_n^a = \mathcal{M}\left(\mathbf{x}_{n-1}^a\right)$, and $\mathbf{x}_n^b = \mathcal{M}\left(\mathbf{x}_{n-1}^b\right)$.

The estimated initial condition $\mathbf{x}_0^a$ (control variable) controls the whole estimated state in space and time for the assimilation time period.

Formulation of NAVDAS-AR …

Euler-Lagrange equations

Analysis $\mathbf{x}^a$ which minimizes J satisfies the following so called Euler-Lagrange (EL) system,

$$\vec{\lambda}_n - \mathbf{M}_n^T \vec{\lambda}_{n+1} = \left\{ \mathbf{H}^T \mathbf{R}^{-1} \left[\mathbf{y} - \mathcal{H}\left(\mathbf{x}^a\right) \right] \right\}_n , \qquad \textbf{(1)}$$

with an initial condition $\vec{\lambda}_{N+1} = 0.$

$$\mathbf{x}_n^a - \mathcal{M}\left(\mathbf{x}_{n-1}^a\right) = \sum_{n'=1}^{N} \mathbf{Q}_{nn'} \vec{\lambda}_{n'} , \qquad \textbf{(2)}$$

with an initial condition $\mathbf{x}_0^a = \mathbf{x}_0^b + \mathbf{P}_0^b \mathbf{M}_0^T \vec{\lambda}_0 .$

Equations (1) – (2) form a nonlinear coupled EL system and cannot be solved with a simple direct integration. An iterative procedure can be used to partially account for the nonlinearity. If $\mathcal{M}$ and $\mathcal{H}$ are linear, however, one can decouple the system using the Representer Method of Bennett (1992).

Formulation of NAVDAS-AR …

Solution to the linear problem (inner loop)

In case of linear $\mathcal{M}$ and $\mathcal{H}$, we can formally write the analysis as,

$$\mathbf{x}^a = \mathbf{x}^b + \mathbf{P}^b\mathbf{H}^T\left[\mathbf{H}\mathbf{P}^b\mathbf{H}^T + \mathbf{R}\right]^{-1}\left[\mathbf{y} - \mathbf{H}\mathbf{x}^b\right]$$
$$= \mathbf{x}^b + \left[\mathbf{H}\mathbf{R}^{-1}\mathbf{H}^T + \left[\mathbf{P}^b\right]^{-1}\right]^{-1}\mathbf{H}^T\mathbf{R}^{-1}\left[\mathbf{y} - \mathbf{H}\mathbf{x}^b\right]$$

1. We first solve the problem $\mathbf{z} = \left[\mathbf{H}\mathbf{P}^b\mathbf{H}^T + \mathbf{R}\right]^{-1}\left[\mathbf{y} - \mathbf{H}\mathbf{x}^b\right]$, the solver.
2. We then post-multiply the solution $\mathbf{z}$ by $\mathbf{P}^b\mathbf{H}^T$, the post-multiplier.
3. Here $\mathbf{P}^b = \mathbf{M}\mathbf{Q}^*\mathbf{M}^T$ or $\mathbf{P}^b = \mathbf{M}\mathbf{M}_0\mathbf{P}_0^b\mathbf{M}_0^T\mathbf{M}^T$ (for perfect model) is a gigantic covariance matrix in space and time and is unknown except for the $\mathrm{I} \times \mathrm{I}$ block $\mathbf{P}_0^b$ at time t_0.
4. $\mathbf{P}^b\mathbf{H}^T$ is the background error covariance between model and observation spaces. $\mathbf{H}\mathbf{P}^b\mathbf{H}^T$ is the background error covariance in the observation-space, is also known as the ***Representer Matrix***. Notice that $\mathbf{P}^b\mathbf{H}^T$ and $\mathbf{H}\mathbf{P}^b\mathbf{H}^T$ can also be estimated using ensemble techniques, such as ExKFs.

Formulation of NAVDAS-AR …

A special matrix/vector multiplication procedure

In both the solver and post-multiplier, we need to evaluate the following matrix/vector multiply operation many times during each inner loop,

$$\mathbf{g} = \left[\mathbf{P}^{b}\mathbf{H}^{T}\right]\mathbf{z}, \qquad (3)$$

where $\mathbf{z}$ is a known vector of length K and $\mathbf{g}$ is a vector of length $N \cdot I$, which is the result of the matrix/vector multiply. Following are the steps to obtain $\mathbf{g}$ through the use of tangent linear and adjoint models.

1. Define $\mathbf{z}^{T} = \left(\mathbf{z}_1 \ldots \mathbf{z}_n \ldots \mathbf{z}_N\right)^{T}$ and $\mathbf{g}^{T} = \left(\mathbf{g}_1 \ldots \mathbf{g}_n \ldots \mathbf{g}_N\right)^{T}$, where $\mathbf{z}_n$ and $\mathbf{g}_n$ are vectors of length k_n and I, respectively. $\mathbf{z}_n$ is assumed to be known for all n.
2. $\mathbf{H}^{T} = \left(\mathbf{H}_1^{T} \ldots \mathbf{H}_n^{T} \ldots \mathbf{H}_N^{T}\right)$ is a $K \times N \cdot I$ block diagonal matrix with N blocks, each of size $k_n \times I$.

Formulation of NAVDAS-AR …

A special matrix/vector multiplication procedure

3. Introduce a vector of length I, $\mathbf{f}_n$ which is defined for each time $\mathbf{t}_n$. Let $\mathbf{f}_n$ be the output from the backward adjoint model, $\mathbf{M}_n^T$, starting at time $\mathbf{t}_N$ and with forcing $\mathbf{H}_n^T\mathbf{z}_n$,

$$\mathbf{f}_n = \mathbf{M}_n^T\mathbf{f}_{n+1} + \mathbf{H}_n^T\mathbf{z}_n, \qquad (4)$$

   subject to $\mathbf{f}_{N+1} = \mathbf{0}$. We refer to (4) as the *backward sweep* which produces a vector $\mathbf{f}_0$ at time $\mathbf{t}_0$.

4. The matrix/vector multiply at time $\mathbf{t}_n$, $\mathbf{g}_n$ is simply the output from the forward tangent linear model, $\mathbf{M}_{n-1}$, starting at time $\mathbf{t}_0$,

$$\mathbf{g}_n = \mathbf{M}_{n-1}\mathbf{g}_{n-1} + \mathbf{Q}_n\mathbf{f}_n, \qquad (5)$$

   subject to $\mathbf{g}_0 = \mathbf{P}_0^b\mathbf{f}_0$. Currently we use a similar procedure as described in Daley and Barker (2000, 2001) to calculate $\mathbf{g}_0$. We refer to (5) as the *forward sweep*.

5. It requires one *single* backward and forward sweep to calculate $\mathbf{P}^b\mathbf{H}^T\mathbf{z}$.

Formulation of NAVDAS-AR …

Solution to the nonlinear problem (outer loop)

In case of nonlinear $\mathcal{M}$ and $\mathcal{H}$, an iterative method is used to partially account for the nonlinearities by solving a sequence of coupled linear EL systems.

Let us introduce an *a priori* state $\left(\mathbf{x}^{\mathrm{p}}\right)^{\mathrm{j}}$ for the j^{th} outer loop iteration, such that $\left(\mathbf{x}^{\mathrm{p}}\right)^{\mathrm{j}}$ is the solution to a linear model that is linearized around the previous analysis $\left(\mathbf{x}^{\mathrm{a}}\right)^{\mathrm{j-1}}$,

$$\left(\mathbf{x}^{\mathrm{p}}\right)_{\mathrm{n}}^{\mathrm{j}} - \mathbf{M}_{\mathrm{n-1}}^{\mathrm{j-1}}\left[\left(\mathbf{x}^{\mathrm{p}}\right)_{\mathrm{n-1}}^{\mathrm{j}} - \left(\mathbf{x}^{\mathrm{a}}\right)_{\mathrm{n-1}}^{\mathrm{j-1}}\right] - \mathcal{M}\left(\left(\mathbf{x}^{\mathrm{a}}\right)_{\mathrm{n-1}}^{\mathrm{j-1}}\right) = \mathbf{0}, \text{ for } 1 \le \mathrm{n} \le \mathrm{N},$$

$$\text{subject to } \left(\mathbf{x}^{\mathrm{p}}\right)_{0}^{\mathrm{j}} = \mathbf{x}_{0}^{\mathrm{b}} \qquad \textbf{(6)}$$

Notice we use the background as the first guess, such that

$$\left(\mathbf{x}^{\mathrm{a}}\right)^{0} = \mathbf{x}^{\mathrm{b}}.$$

Formulation of NAVDAS-AR …

Solution to the nonlinear problem (outer loop)

The analysis for the j^{th} iteration, $\left(\mathbf{x}^{a}\right)^{j}$, may now be written as,

$$\left(\mathbf{x}^{a}\right)^{j}=\left(\mathbf{x}^{p}\right)^{j}+\left(\mathbf{P}^{b}\right)^{j\text{-}1}\left[\mathbf{H}^{j\text{-}1}\right]^{T}\boldsymbol{\beta}^{j}$$

where,

$$\boldsymbol{\beta}^{j}=\left[\mathbf{H}^{j-1}\left(\mathbf{P}^{b}\right)^{j\text{-}1}\left[\mathbf{H}^{j-1}\right]^{T}+\mathbf{R}\right]^{-1}\left[\mathbf{y}-\mathcal{H}\left(\left(\mathbf{x}^{a}\right)^{j\text{-}1}\right)-\mathbf{H}^{j\text{-}1}\left[\left(\mathbf{x}^{p}\right)^{j}-\left(\mathbf{x}^{a}\right)^{j\text{-}1}\right]\right]$$

and,

$$\left(\mathbf{P}^{b}\right)^{j\text{-}1}=\mathbf{M}^{j\text{-}1}\mathbf{Q}^{*}\left[\mathbf{M}^{j\text{-}1}\right]^{T},$$

for a perfect model,

$$\left(\mathbf{P}^{b}\right)^{j\text{-}1}=\mathbf{M}^{j\text{-}1}\mathbf{M}_{0}^{j\text{-}1}\mathbf{P}_{0}^{b}\left[\mathbf{M}_{0}^{j\text{-}1}\right]^{T}\left[\mathbf{M}^{j\text{-}1}\right]^{T}.$$

Summary:

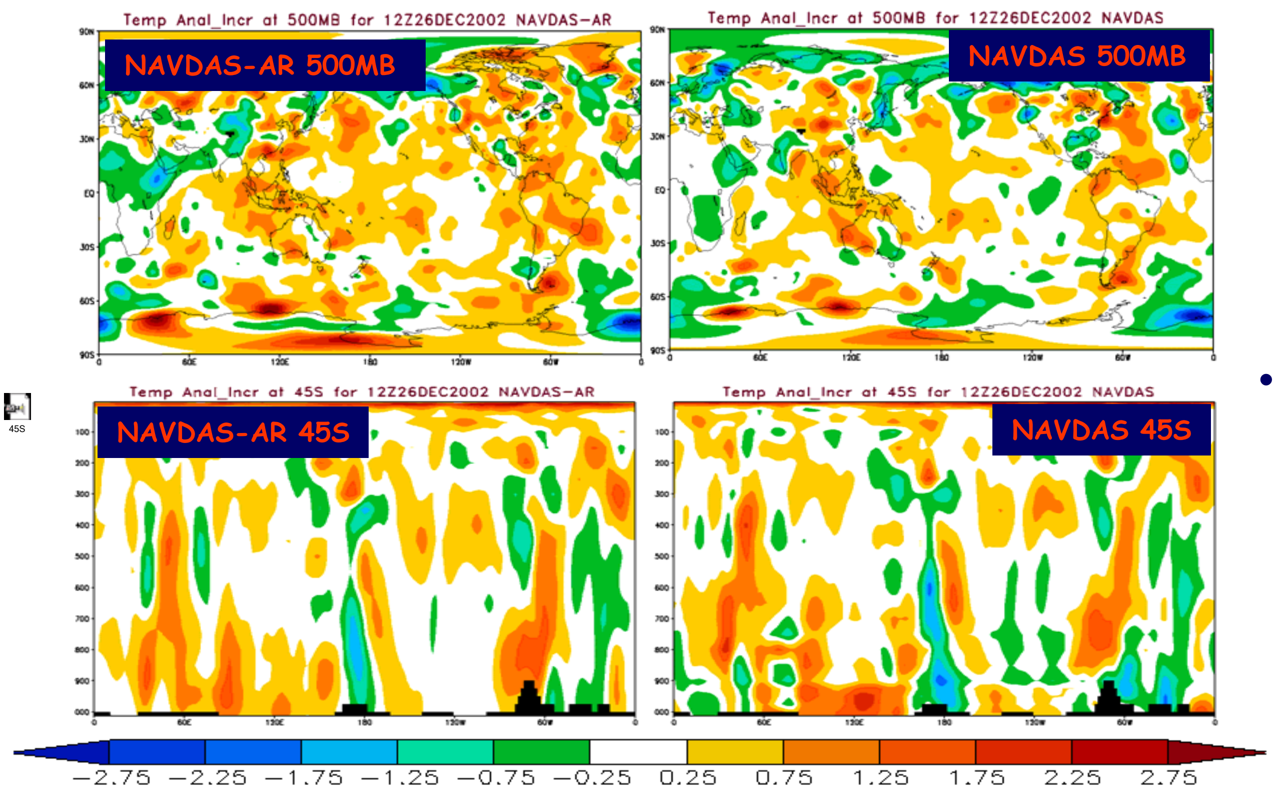
- A linear prediction model is used to generate background to be used for the inner loop in each subsequent outer iteration.
- The initial condition for each subsequent background is always the same.

Building Blocks of NAVDAS-AR

- **Nonlinear and linearized NOGAPS:**
  - Nonlinear NOGAPS is used in first outer loop to provide the trajectories for innovation calculation and the TLM/Adjoint models.
  - Linearized NOGAPS is used in subsequent outer loops to provide these trajectories
- **Adjoint and tangent linear (TLM) of NOGAPS:**
  - Evolve innovations (Adjoint) and analysis increments (TLM) in time.
- **Observation operators and associated Jacobians:**
  - Used to calculate/recalculate the innovation vector.
- **A preconditioned Conjugate Gradient (CG) solver:**
  - Perform the inner-loop minimization.
- **Error covariance specifications/models:**
  - Control the outcome of data assimilation.

Initial Test of the Inner Loop

Assimilation 09Z – 15Z 26DEC2002
Temperature Analysis Corrections at 12Z

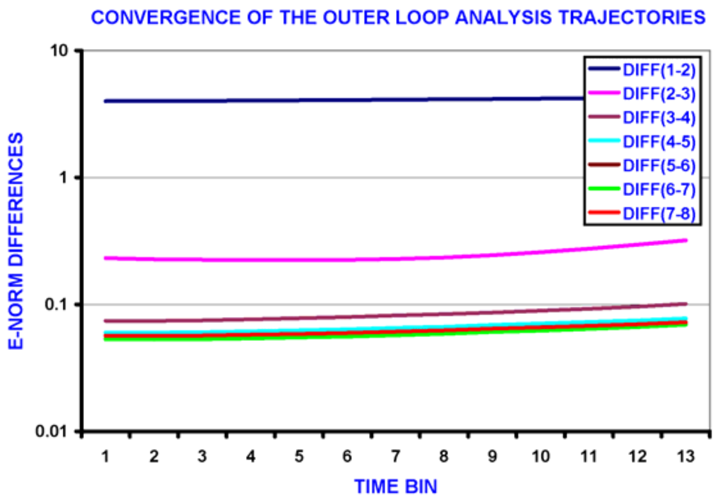


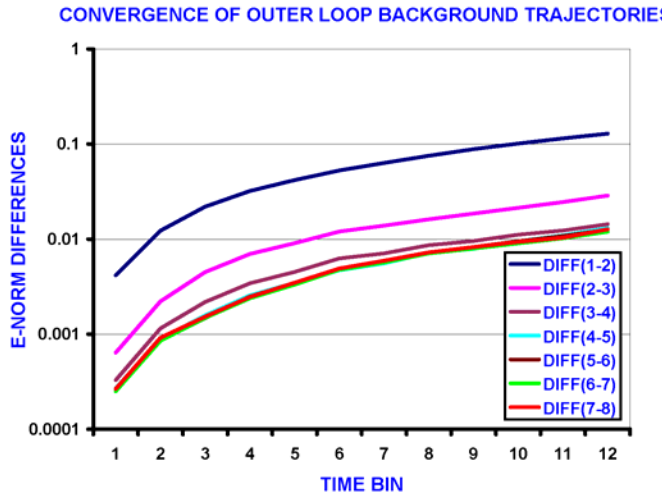
- **Observations: A NAVDAS innovation vector (~400,000 observations) was used in both runs except that the observations are binned in half hour bins in NAVDAS-AR run. (NAVDAS-AR was designed to use the existing NAVDAS infrastructure.)**
- **Dynamic model and background: A T47L30 NOGAPS was used as the forecast and tangent-linear models. A perfect model assumption, though not required, was used in these experiments.**

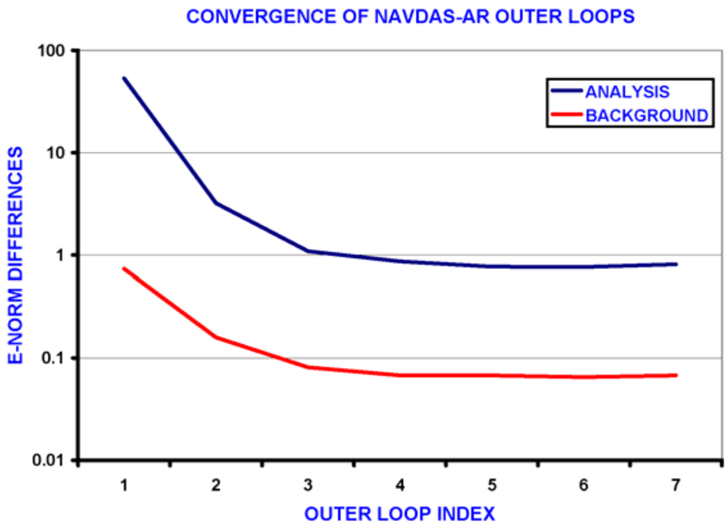
•NAVDAS COST $O(N^2)$, **N= ob #**

•NAVDAS-AR COST *F***(Inner loop model resolution) +** $O(N)$

Initial Test of the Outer Loop



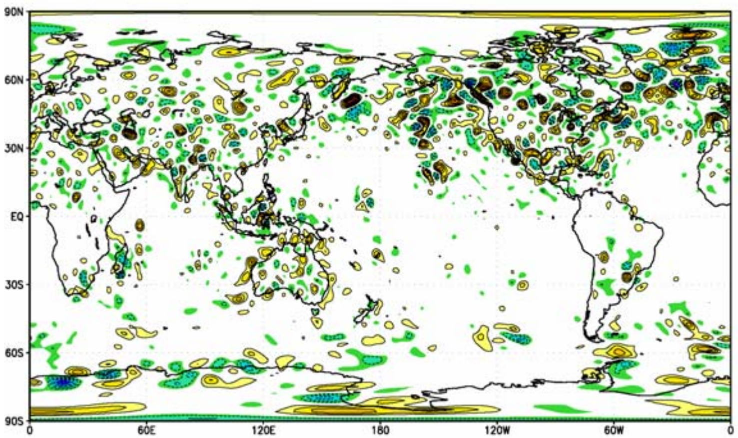




- A new procedure to treat the non-linearity in NAVDAS-AR has been implemented and tested.
- Eight outer loops were used to examine the convergence property.
- The preliminary results suggested that the outer loop converges after 3 iterations.

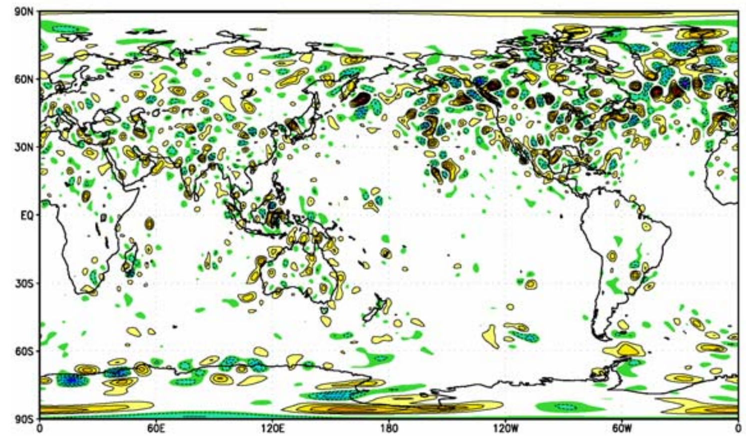
Convergence of the Outer Loops

VORTICITY AT 500.0 MBS(ANALINC) : 2004031200



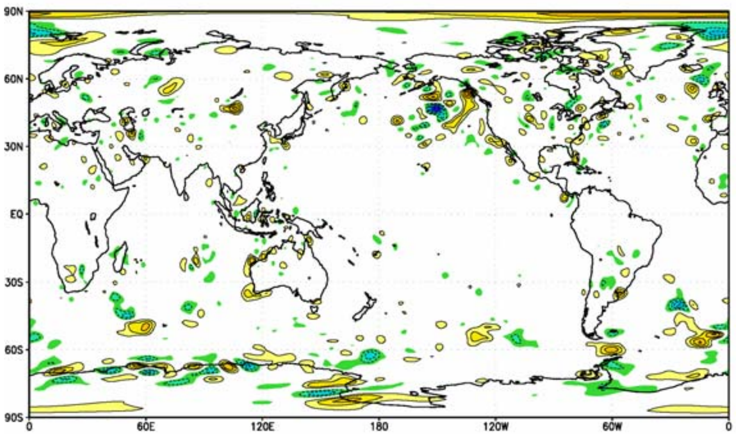
DIFFERENCE PLOT : CDATA1–CDATA2

VORTICITY AT 500.0 MBS(ANALINC) : 2004031200

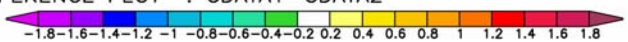


DIFFERENCE PLOT : CDATA1–CDATA6

VORTICITY AT 1000.0 MBS(ANALINC) : 2004031200



DIFFERENCE PLOT : CDATA1–CDATA2



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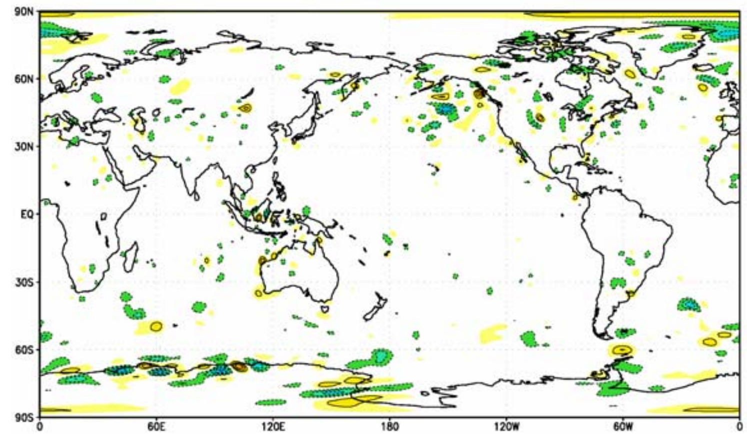

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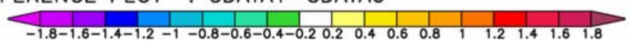
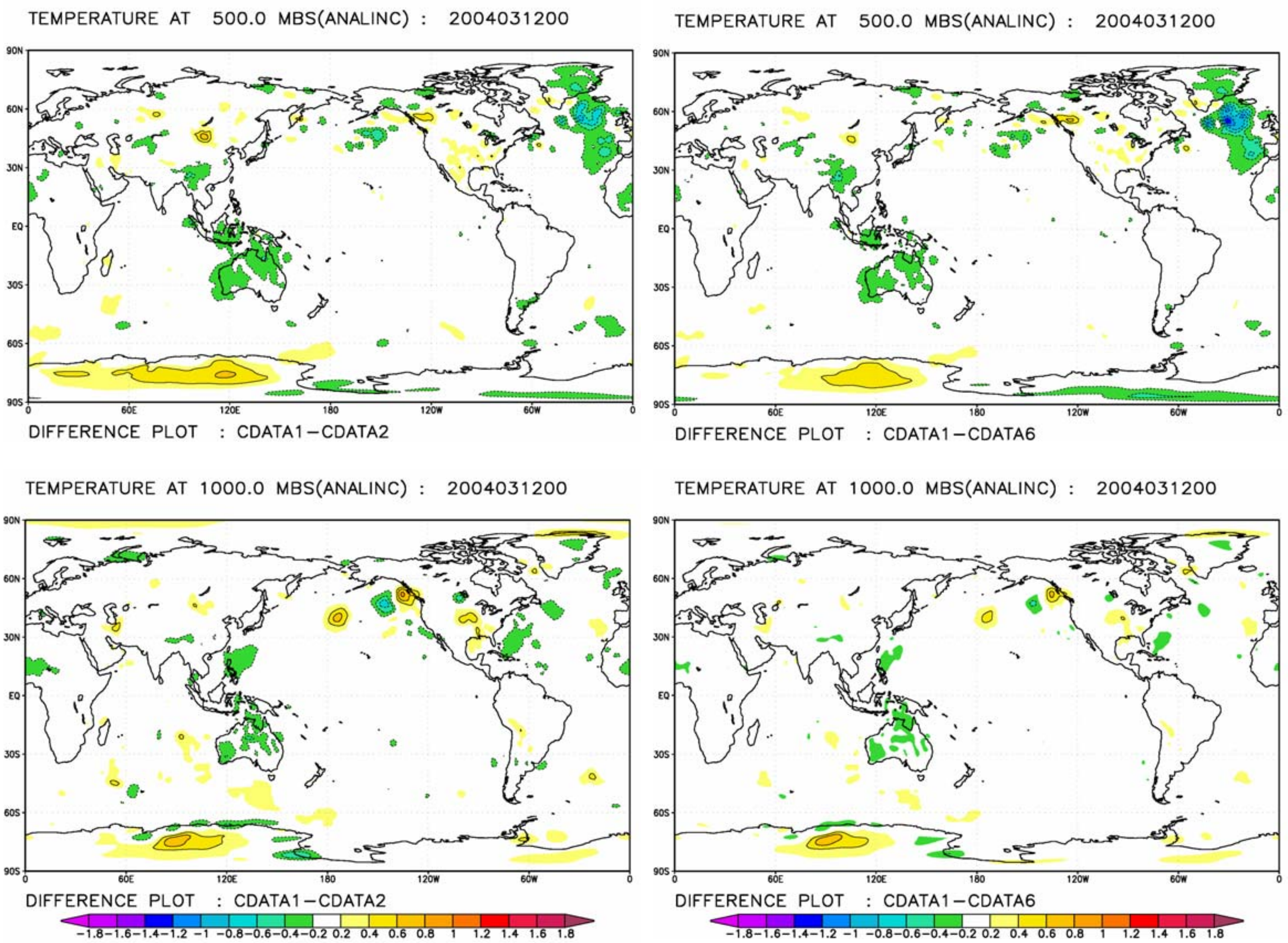


- Nonlinear and Linear NOGAPS (first guess & trajectory) at T239L30
- Tangent linear and adjoint NOGAPS (minimization) at T79L30
- Only conventional observations were assimilated
- Impact of the nonlinearity in NOGAPS
- Majority corrections happened in the first 2 outer loops

Convergence of the Outer Loops …



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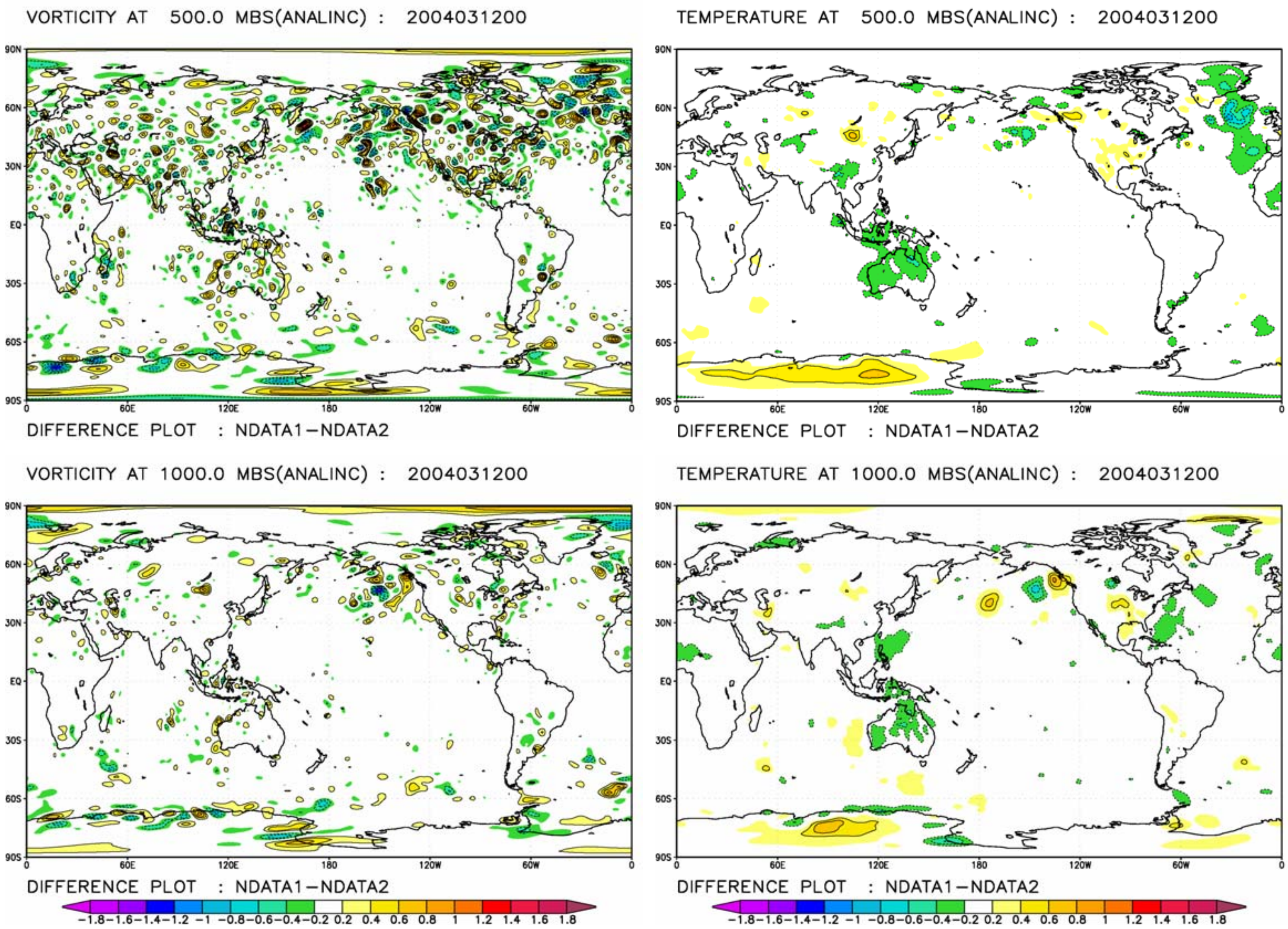
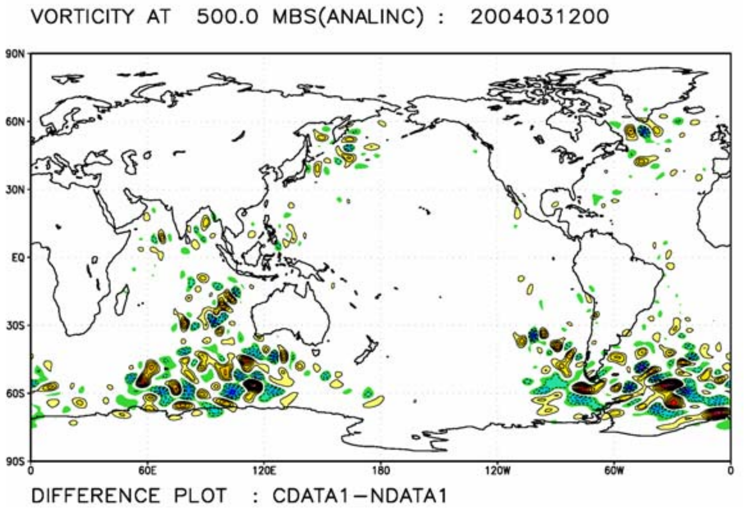
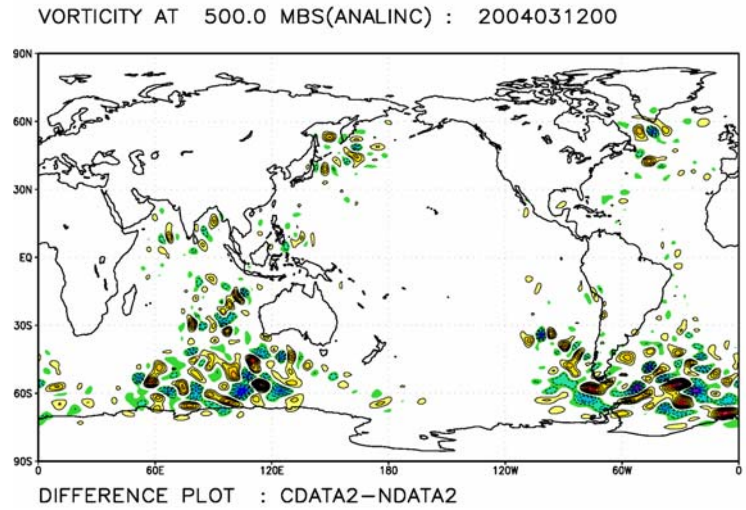
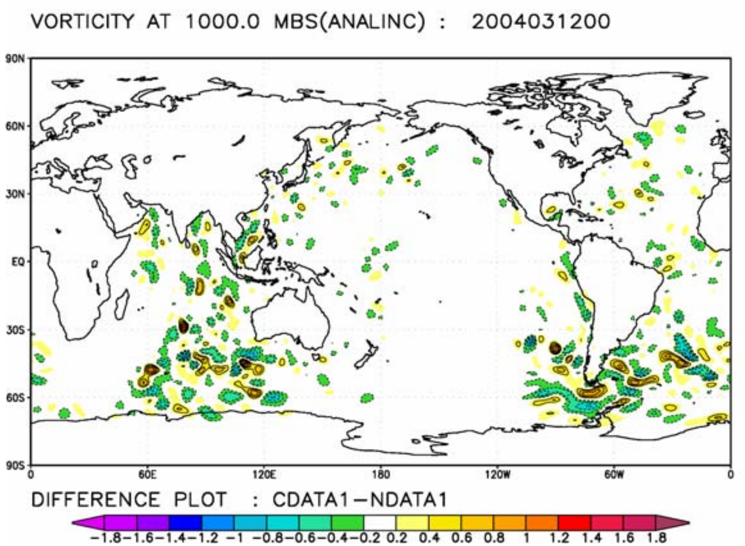


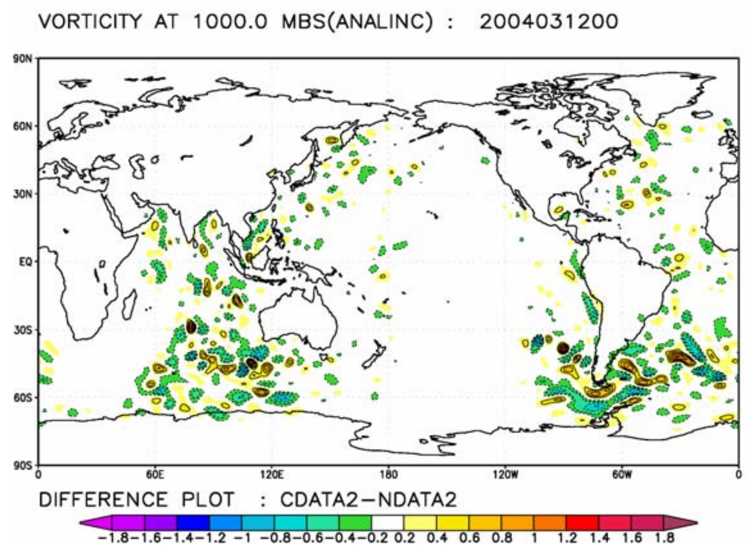
- Nonlinear and Linear NOGAPS at T239L30
- Tangent linear and adjoint NOGAPS at T79L30
- Conventional observations + SSM/I wind speeds and TPW were assimilated
- Nonlinearities in NOGAPS and in SSM/I windspeeds and TPW

Impact of SSM/I Windspeeds and TPW …



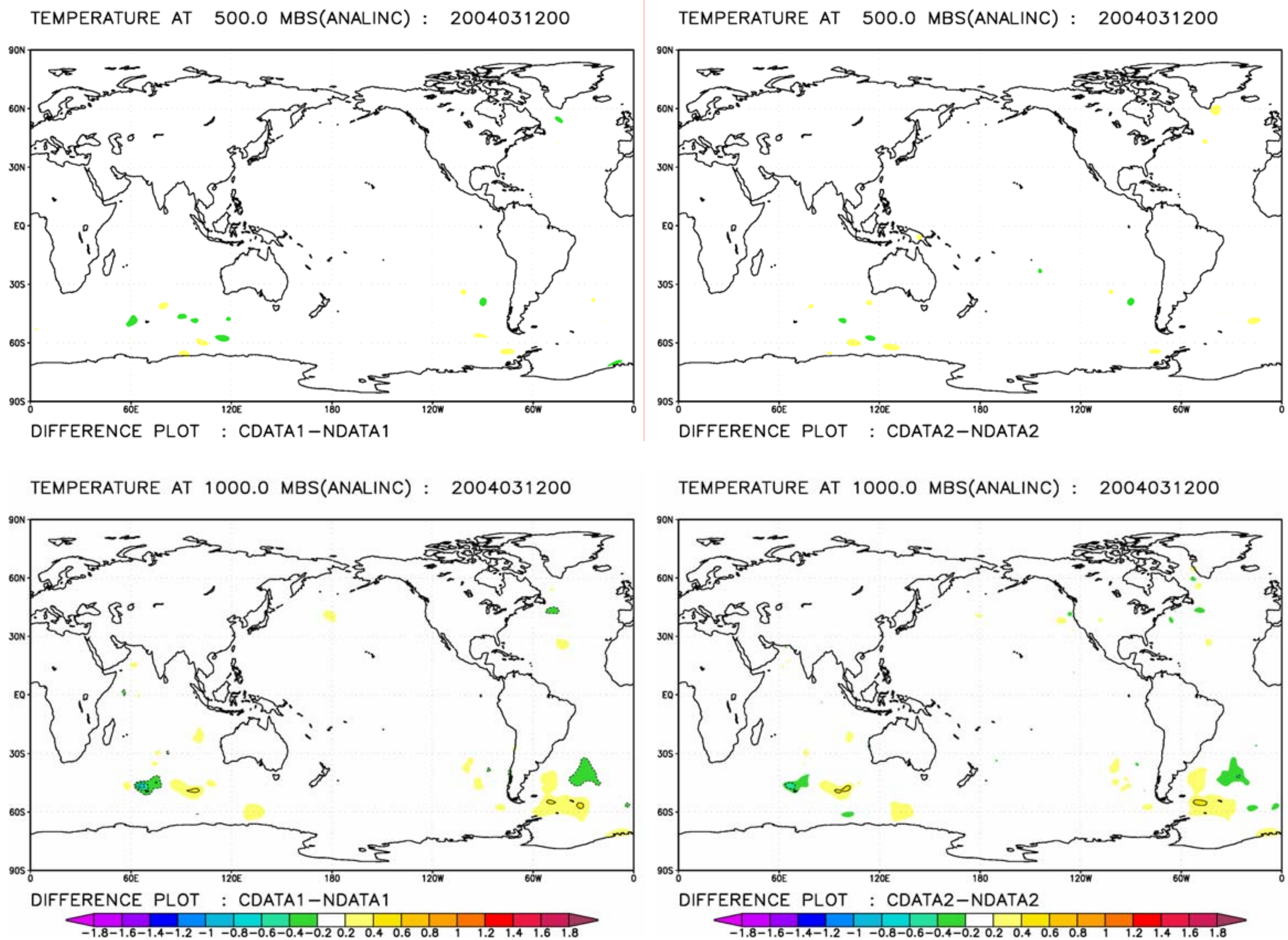






- **Vorticity difference between no-SSM/I and with-SSM/I**
- **Majority of the differences occurred along the satellite path and over the Southern Hemisphere**

Impact of SSM/I Windspeeds and TPW …



- **Temperature difference between no-SSM/I and with-SSM/I**
- **Majority of the differences occurred along the satellite path near the surface over the Southern Hemisphere**

Issues and Opportunities

- **Issues:**
  - A preconditioner for the CG solver using the Lanczos connection
  - A more efficient convolution of initial background error covariance with the adjoint sensitivity at the initial time
  - Updating flow-dependent initial background error covariance in a cycling operational environment
  - Accurate, efficient, and portable observation operators and the associated Jacobians and their adjoints
  - Including impact of model errors
- **Opportunities:**
  - Study impact of new sensors on analysis using NAVDAS-AR.
  - Examine four-dimensional observation sensitivity using the adjoint of NAVDAS-AR.

Concluding Remarks

- We have formulated and constructed a natural four dimensional follow-on to NAVDAS, NAVDAS-AR, which was initiated by Roger Daley at NRL.
- The minimization component (inner loop) to the linear case has been developed and the results of initial testing are encouraging.
- A new iterative procedure (outer loop) to account for some of the nonlinearity in prediction model and observation operators has be developed and tested.
- Impact of model error needs to be properly treated and studied.
- Help is needed in terms of observation operators and the associated TLM and adjoints.

Thank You

Extra Slides

Definition of $\mathbf{M}^{j\text{-}1}$

Let,

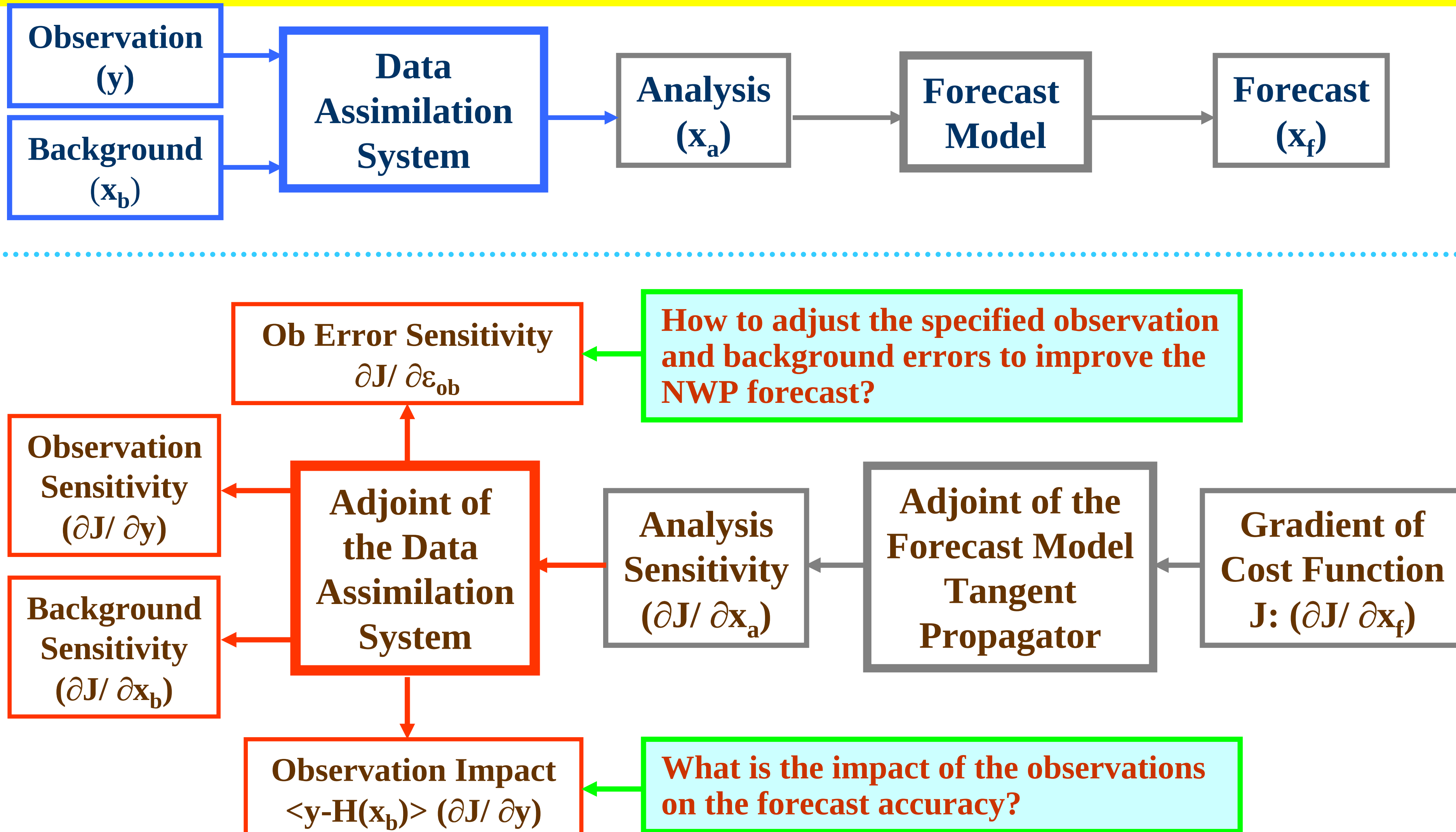
$$\mathbf{M}^{j\text{-}1} = \begin{pmatrix} \mathbf{I} & . & . & . & . & \mathbf{0} \\ \prod_{n'=1}^{1} \mathbf{M}_{n'}^{j\text{-}1} & \mathbf{I} & . & . & . & . \\ . & . & . & . & . & . \\ \prod_{n'=n-1}^{1} \mathbf{M}_{n'}^{j\text{-}1} & . & \prod_{n'=n-1}^{n-1} \mathbf{M}_{n'}^{j-1} & \mathbf{I} & . & . \\ . & . & . & . & . & . \\ \prod_{n'=N-1}^{1} \mathbf{M}_{n'}^{j\text{-}1} & . & . & . & \prod_{n'=N-1}^{N-1} \mathbf{M}_{n'}^{j\text{-}1} & \mathbf{I} \end{pmatrix}.$$

Definition of $\left(\mathbf{Q}^{*}\right)^{\mathrm{j-1}}$

Let,

$$
\left(\mathbf{Q}^{*}\right)^{\mathrm{j-1}} = \begin{pmatrix}
\mathbf{M}_0^{\mathrm{j-1}}\mathbf{P}_0^{\mathrm{b}}\left[\mathbf{M}_0^{\mathrm{j-1}}\right]^{\mathrm{T}} + \mathbf{Q}_1 & \mathbf{0} & . & . & . & . & \mathbf{0} \\
\mathbf{0} & \mathbf{Q}_2 & \mathbf{0} & . & . & . & . \\
 & & & . & & & \\
. & & & \mathbf{Q}_n & \mathbf{0} & . & . \\
. & & & . & & & \\
. & . & . & . & \mathbf{0} & \mathbf{Q}_{n-1} & \mathbf{0} \\
\mathbf{0} & . & . & . & . & \mathbf{0} & \mathbf{Q}_N
\end{pmatrix}
$$

NAVDAS Adjoint System



Baker and Langland

Observation and Background Sensitivity

$$\partial \mathrm{J} / \partial \mathbf{y} = \left(\mathbf{HP}^{\mathrm{b}} \mathbf{H}^{\mathrm{T}} + \mathbf{R} \right)^{-1} \mathbf{HP}^{\mathrm{b}} \partial J / \partial \mathbf{x}^{\mathrm{a}}$$

$$\partial \mathrm{J} / \partial \mathbf{x}^{\mathrm{b}} = \left[\mathbf{I} - \mathbf{H}^{\mathrm{T}} \left(\mathbf{HP}^{\mathrm{b}} \mathbf{H}^{\mathrm{T}} + \mathbf{R} \right)^{-1} \mathbf{HP}^{\mathrm{b}} \right] \partial J / \partial \mathbf{x}^{\mathrm{a}}$$