# Recent developments in the use and understanding of adjoint-derived estimates of observation impact

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## 1 Introduction

During the last several years, the adjoint of a data assimilation system has emerged as an accurate and efficient tool for estimating observation impacts on short-range weather forecasts (Langland and Baker 2004, Gelaro et al. 2007, Cardinali 2009). With this tool, the impacts of any or all observations can be computed simultaneously based on a single execution of the adjoint system. In addition, the results can be easily aggregated by data type, location, channel, etc., making this technique especially attractive for regular, even near-real time, monitoring of the entire observing system. Currently the adjoint approach is used at several forecast centers either for experimentation or routine monitoring of observation impacts on short-range forecasts. Also, a coordinated experiment is being conducted to compare adjoint-based estimates of observation impacts produced in different forecast systems.

In this paper we review recent developments in the use of the adjoint technique for estimating observation impact and interpretation of the results obtained. Results from the aforementioned comparison project are shown for the forecast systems used at the Naval Research Laboratory (NRL) and NASA Global Modeling and Assimilation Office (GMAO). In addition, we review key findings from ongoing research with the adjoint method, including the need for and implications of greater-than-first-order estimates of impact, extension of the method to nonlinear analysis problems, and the comparison of adjoint-based estimates of observation impact with those derived from traditional observing system experiments (OSEs).

## 2 Estimation of observation impact

A technique for using the adjoint of a data assimilation system to measure observation impact was proposed by Langland and Baker (2004, hereafter LB04). It efficiently estimates the impact of individual observations on an energy-based measure of forecast error

$$e = (\mathbf{x}^f - \mathbf{x}^t)^{\mathrm{T}}\mathbf{P}^{\mathrm{T}}\mathbf{C}\,\mathbf{P}\,(\mathbf{x}^f - \mathbf{x}^t)\,, \tag{1}$$

where $\mathbf{x}^f$ is a forecast state, $\mathbf{x}^t$ is a verification state (considered 'truth'), $\mathbf{C}$ is a diagonal matrix of weights that gives (1) units of energy per unit mass (J/kg), $\mathbf{P}$ is a spatial projection operator that measures $e$ only within a specified region of interest and the superscript T denotes the transpose operation. The measure of observation impact is taken to be the difference in $e$ between forecasts initialized from an analysis $\mathbf{x}_a$ and corresponding background state $\mathbf{x}_b$, where this difference is due entirely to the assimilation of the observations. It can be expressed in the form

$$\delta e = \langle \mathbf{K}^{\mathrm{T}}\mathbf{g}, \mathbf{d}\rangle\,, \tag{2}$$

where $\mathbf{K}^{\mathrm{T}}$ is the adjoint of the analysis scheme, $\mathbf{g}$ is a vector in model space (described below) that includes sensitivity information produced by the adjoint of the forecast model and $\mathbf{d}$ is the vector of observation-minus-background departures (innovations) used to produce the analysis

$$\mathbf{x}_a = \mathbf{x}_b + \mathbf{K}\mathbf{d}. \tag{3}$$

In general, computation of the innovations requires an observation operator, $H$, that relates the model state to the observations, $\mathbf{y}$, such that $\mathbf{d} = \mathbf{y} - H(\mathbf{x})$. In (2) and (3), it is assumed that $H$ is either linear or a function of only $\mathbf{x}_b$, although this is not necessarily true in general. This is discussed further in section 2.2.

The expression (2) represents a weighted sum of the innovations for all assimilated observations. The impact of a particular subset of observations may be quantified by summing only those terms in (2) involving the corresponding elements of $\mathbf{d}$. The computation of $\mathbf{K}^{\mathrm{T}}\mathbf{g}$ is done only once, however, based on the complete set of observations. Thus, the impact of a given subset of observations is determined with respect to all other observations *simultaneously*. This contrasts with traditional OSEs that estimate the forecast impact for subsets of observations that are withheld from (or added to) the analysis in a series of separate experiments. The computational cost of producing the observation impact information using the adjoint system is about the same as re-runnning the (forward) analysis and forecast model, although this can be reduced depending on the method used to compute $\mathbf{K}^{\mathrm{T}}$ (Trémolet 2008).

## 2.1 Orders of approximation of $\delta e$

As derived by LB04, $\mathbf{g}$ has the form

$$\mathbf{g} = \mathbf{M}_b^{\mathrm{T}}\mathbf{P}^{\mathrm{T}}\mathbf{C}\,\mathbf{P}\,(\mathbf{x}_b^f - \mathbf{x}^t) + \mathbf{M}_a^{\mathrm{T}}\mathbf{P}^{\mathrm{T}}\mathbf{C}\,\mathbf{P}\,(\mathbf{x}_a^f - \mathbf{x}^t)\,, \tag{4}$$

where $\mathbf{x}_b^f$ and $\mathbf{x}_a^f$ are forecasts initialized from $\mathbf{x}_b$ and $\mathbf{x}_a$, and $\mathbf{M}_b^{\mathrm{T}}$ and $\mathbf{M}_a^{\mathrm{T}}$ represent the adjoint of the forecast model evaluated along those trajectories. Errico (2007) placed (2) in the context of various-order Taylor series approximation of $\delta e$ in terms of $\mathbf{d}$, whose order depends on the form of $\mathbf{g}$. The expression in (4), is that of a non-linear (essentially third-order) approximation of $\delta e$.

Owing to the quadratic nature of (1), an approximation beyond first order is indeed required to obtain a sufficiently accurate estimate of $\delta e$ (Gelaro et al. 2007). Fig. 1 compares the first-, second- and third-order approximations of $\delta e$ with the "actual" difference, $e(\mathbf{x}_a^f) - e(\mathbf{x}_b^f)$, computed in physical space from a series of 24-hour forecasts and verifying analyses at 00 UTC for each day during July 2005. The results were produced using forward and adjoint versions of the NASA GEOS-5 atmospheric data assimilation system, including all conventional observations and satellite radiances assimilated operationally at the time. Note first that $\delta e$ is negative for all days, indicating that the assimilation of the complete set of observations consistently results in a more accurate 24-hour forecast. The first-order approximation clearly overestimates the beneficial impact of the observations, by roughly a factor of two. This is an expected result provided $\mathbf{x}_a$ is close to the minimum of $e$ (Trémolet 2007). The second- and third-order approximations are much more accurate; they lie within approximately 15% of the actual values overall. The fact that the higher-order approximations still slightly underestimate the beneficial impact of the observations is mostly likely due to deficiencies associated with the adjoint forecast model, including the absence of moist physical processes present in the nonlinear forecast model.

Whereas (4) is a function of both $\mathbf{x}_b$ and $\mathbf{x}_a$, its first-order counterpart is a function of $\mathbf{x}_b$ only (not shown). Consequently, the former generally depends on all the elements of $\mathbf{d}$ through $\mathbf{x}_a$, as implied by (3). As pointed out by Errico (2007), the necessity of using greater-than-first-order approximations of $\delta e$ to obtain accurate estimates of observation impact means that partial sums used to quantify the impact of a particular subset of observations may be somewhat ambiguous since such sums involve cross-products with innovations outside the set in question. Gelaro et al. (2007) found this effect to be apparently small when measuring the impacts of

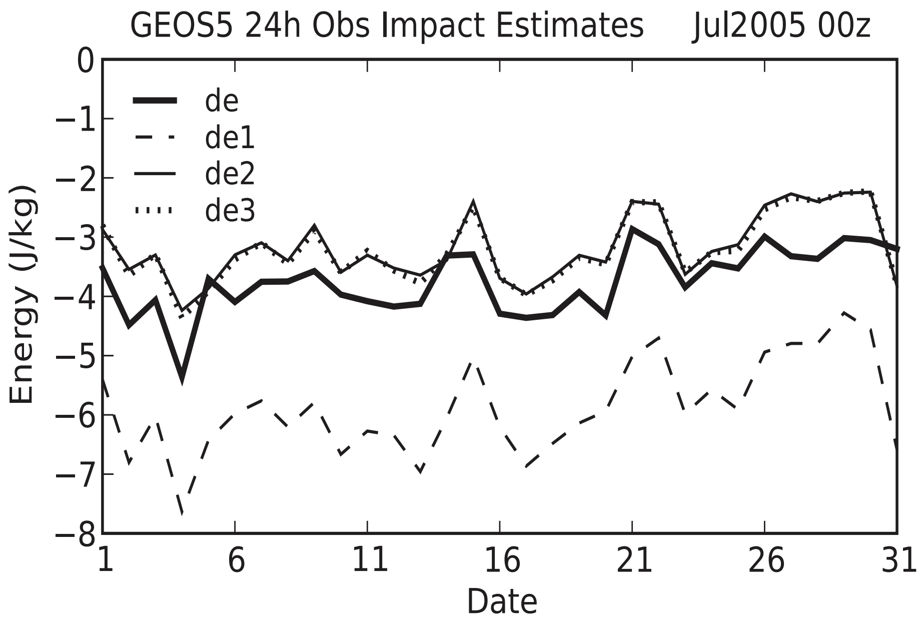


*Figure 1: Time series of forecast error reduction, $\delta e$, due to assimilation of observations in GEOS-5 during July 2005 computed from the model fields directly (thick solid), and estimated using the adjoint-based first-order approximation, $\delta e_1$ (dash), second-order approximation, $\delta e_2$ (thin solid) and third-order approximation, $\delta e_3$ (dotted) (Gelaro et al. 2007).*

large subsets of observations on global-scale measures of $e$. It has not been shown that this effect is negligible in general.

### 2.2 Nonlinear analysis problems

In variational data assimilation systems such as those used at most operational forecast centers, the analysis cost function is nonlinear and difficult to minimize. Typically, a Gauss-Newton procedure is used to minimize an approximate quadratic cost function defined by linearizing $H$ around the current state estimate, where the analysis increment is the control variable of the problem. The process is repeated until a satisfactory solution is found, and these repeated minimizations define the so-called outer loops of an incremental variational data assimilation scheme (Courtier et al. 1994). In such a scheme, the analysis increment is not $\mathbf{x}_a - \mathbf{x}_b = \mathbf{K}\mathbf{d}$ as given by (3), but rather, after loop $j$,

$$\mathbf{x}_j - \mathbf{x}_b = \mathbf{K}_j\mathbf{d}_j + \mathbf{K}_j\mathbf{H}_j(\mathbf{x}_{j-1} - \mathbf{x}_b)\,, \tag{5}$$

where $\mathbf{d}_j = \mathbf{y} - H(\mathbf{x}_{j-1})$ and $\mathbf{H}_j$ is the observation operator linearized around the (previous) state estimate $\mathbf{x}_{j-1}$.

Trmolet (2008) examined the computation of observation impact in an incremental data assimilation system with multiple outer loops. He showed that, while the second-order adjoint of the assimilation system is required to account fully for the impact of the outer loops (which is not practical in a realistic system), a partial treatment of their effects is possible with certain approximations. These include neglecting second-order terms that contain information about the sensitivity of the operators in (5) with respect to the state estimate, which may be important, especially in four-dimensional variational (4D-Var) assimilation. Nonetheless, by applying (5)

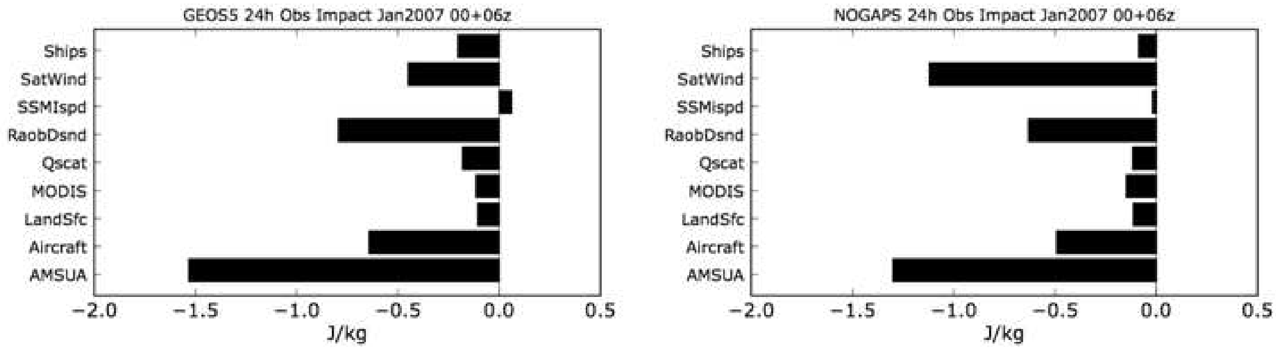


*Figure 2: Daily average impact of various observing systems on 24-h forecasts from 00+06UTC in GEOS-5 (left) and NOGAPS (right) during January 2007. Negative values indicate forecast error reduction.*

recursively, the total increment can be written as a linear combination of the observation departures from the various intermediate state estimates, and the impact of observations (on the measure $e$) can be estimated by the scalar product

$$I = \sum_{j=1}^{m} \langle \mathbf{K}_j^{\mathrm{T}} \mathbf{L}_j^{\mathrm{T}} \mathbf{g}, \mathbf{d}_j \rangle \,, \tag{6}$$

where $\mathbf{L}_j = \mathbf{K}_m \mathbf{H}_m \ldots \mathbf{K}_{j+1} \mathbf{H}_{j+1}$, $\mathbf{L}_m = \mathbf{I}$ and $m$ is the total number of outer loops.

In the following section we present observation impact results for a system with $m = 2$ outer loops which, based on (6), is computed as

$$I = \langle \mathbf{K}_1^{\mathrm{T}} \mathbf{H}_2^{\mathrm{T}} \mathbf{K}_2^{\mathrm{T}} \mathbf{g}, \mathbf{d}_1 \rangle + \langle \mathbf{K}_2^{\mathrm{T}} \mathbf{g}, \mathbf{d}_2 \rangle \,. \tag{7}$$

Note that the departures in the last (second) outer loop are weighted only by the corresponding operators for this loop. This term is similar in form to that in (2) for the linear analysis problem, or equivalently an analysis produced using a single outer loop. In contrast, the departures in the preceding (first) outer loop are weighted by the operators corresponding to that loop, as well as those in successive outer loops.

## 3 Results from a recent inter-comparison project

An experiment is being conducted to directly compare observation impacts in different forecast systems using the adjoint method. Here, we present results for a baseline set of observations used by two global forecast systems for the month of January 2007. The systems are NAVDAS-NOGAPS (NRL-Monterey) and GEOS-5 (NASA). It is anticipated that the final set of results will also include contributions from the ECMWF and Canadian global models.

The baseline set of observations is defined as those observation types used in common by all forecast systems of the participating institutions during January 2007. It includes AMSU-A radiances in addition to conventional observations and satellite atmospheric motion vectors (AMVs), but does not include more recent observation types such as AIRS and IASI. The latter will be included in future comparisons. For some observation types there are differences in the number and exact criteria for how data are selected for each forecast system. For example, NOGAPS uses a larger number of AMVs, while GEOS-5 uses a larger number of AMSU-A radiances.

The measure $e$ is defined as the dry total energy of the 24-h forecast error between the surface and about 150 hPa over the global domain. The adjoint versions of the forecast models in this experiment are run in dry mode

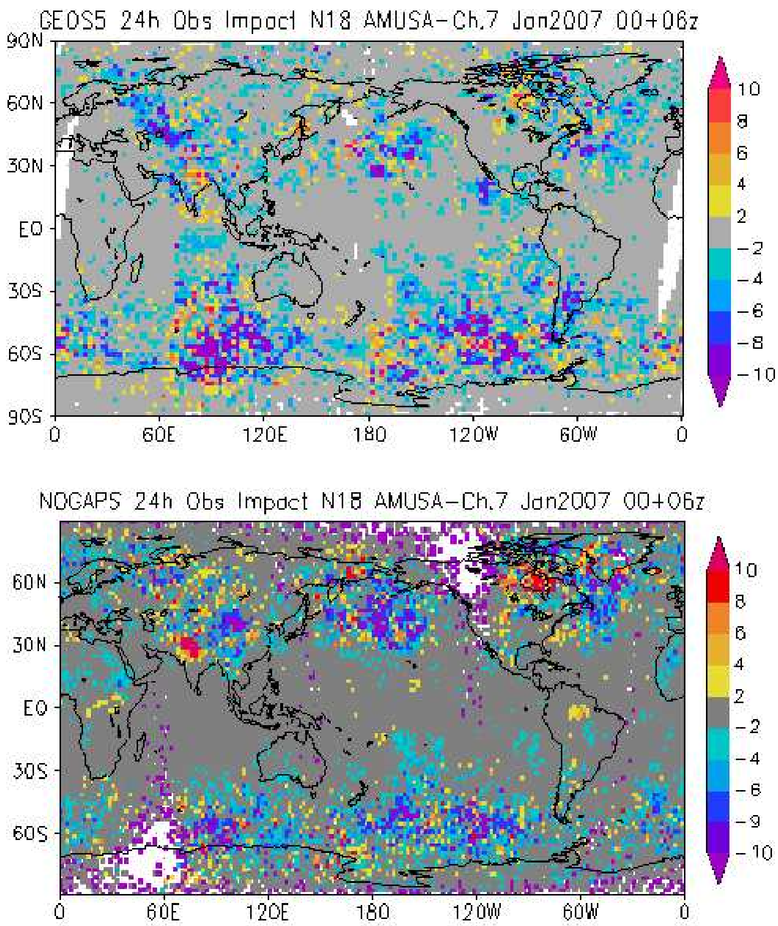


*Figure 3: Impact of NOAA-18 AMSU-A channel 7 brightness temperatures on 24-h forecasts from 00+06UTC in GEOS-5 (top) and NOGAPS (bottom) during January 2007. The units are J/kg. Negative values indicate forecast error reduction.*

with no moist physics. The NOGAPS adjoint is run at T239L30 resolution (identical to the forecast model), and the GEOS-5 forecast model adjoint is run at 1.0-degree resolution (half that of the forecast model).

Both NAVDAS and the GEOS-5 data assimilation system adjoints are 3D-Var schemes with roughly 0.5-degree resolution. NAVDAS is an observation-space, linear analysis algorithm, so that observation impact is computed as in (2). GEOS-5 uses a model-space, incremental variational analysis algorithm with two outer loops based on the Gridpoint Statistical Interpolation scheme (GSI, Wu et al. 2002). Observation impact in GEOS-5 is thus computed as in (7).

In the baseline experiment, we have calculated adjoint-based observation impact at every analysis time (00, 06, 12, 18UTC) for the month of January 2007, which provides 124 sets of results. We show here three figures to illustrate results. Fig. 2 displays the daily average observation impact (00+06UTC) in GEOS-5 and NOGAPS for nine categories of observations. In both GEOS-5 and NOGAPS, the largest total impact for this baseline set of observations is provided by AMSU-A radiances. Large impacts in both systems are also provided by AMVs, radiosondes, and commercial aircraft. It can be noted that the impact of these four observation types (radiances, AMVs, radiosondes, and commercial aircraft) also provide the largest observation impacts in the operational NOGAPS-NAVDAS, which is monitored on a routine basis in both 3d-VAR and 4d-VAR versions.

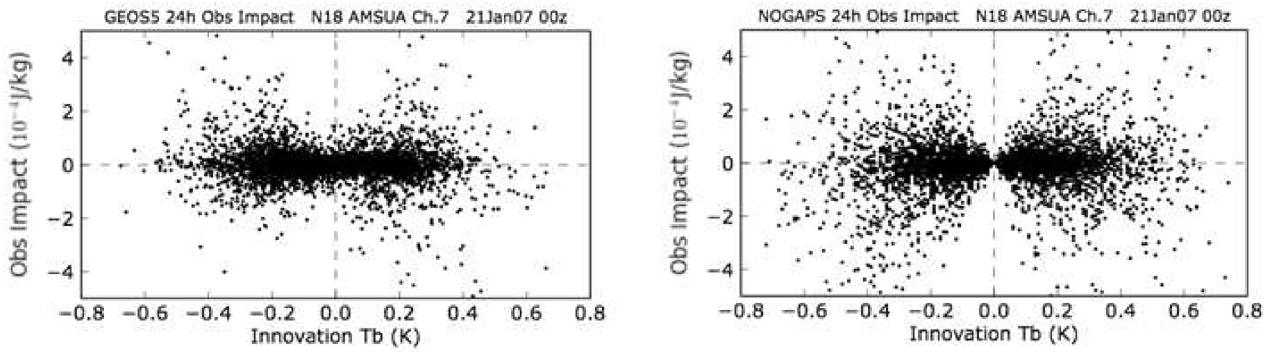


*Figure 4: Scatter diagram of observation impact versus innovation (departure) for NOAA-18 AMSU-A channel 7 brightness temperatures for the 24-h forecast initialized 00UTC 21 January 2007 in GEOS-5 (left) and NOGAPS (right).*

The dominance of these four observation types is therefore a very robust result, confirming that they were the backbone of the global atmospheric observing network during this time. The impact of AMVs is substantially larger in NOGAPS, which assimilates considerably more of this observation type. The remaining observation types—ship and land surface, MODIS, and QuikScat—provide smaller impacts individually, but their combined impact is significant. There is a small error reduction from SSMI wind speeds in NOGAPS and a moderate error increase from this observation type in GEOS-5.

Fig. 3 illustrates the capability of the adjoint method to quantify the impact of specific instrument observation subsets, in this case for NOAA-18 AMSU-A radiance channel 7, which provides large forecast error reduction in both GEOS-5 and NOGAPS. Similar maps can be made for any selected instrument or satellite channel. Note in Fig. 3 the large error reductions provided over the southern hemisphere, and the northern hemisphere oceans. Interestingly, non-beneficial impact from these radiances occurs over parts of India and central Canada in both GEOS-5 and NOGAPS. This could be caused by land or ice-surface contamination of the processed radiance observations, and indicates the utility of this method for identifying possible problems with observation quality or data assimilation procedures.

Fig. 4 shows how the adjoint method allows observation impact to be diagnosed in the context of other fundamental aspects of the assimilation scheme such as the distribution of the innovations (or departures). Here we show scatter diagrams of the impacts of channel 7 brightness temperatures from NOAA-18 AMSU-A as a function of the departures for the forecast initiated at 00UTC on 21 January. Two aspects are revealed that appear to be fundamental to both (and most likely all) forecast systems. The first is that the numbers of observations providing beneficial (negative ordinate values) and non-beneficial (positive ordinate values) impact are both large. In fact, it turns out that only a small majority of the total number of observations of all types—roughly 50-54% on average—are beneficial, although this small majority provides the overall benefit provided by the assimilation as revealed for example in Fig. 2. The second aspect revealed by close inspection of Fig. 4 is that most of the total forecast error reduction comes from observations with moderate-size innovations providing moderate-size reductions, and not from outliers with very large positive or negative innovations. Both aspects may help inform future strategies for data selection and other aspects of optimizing the use of observations.

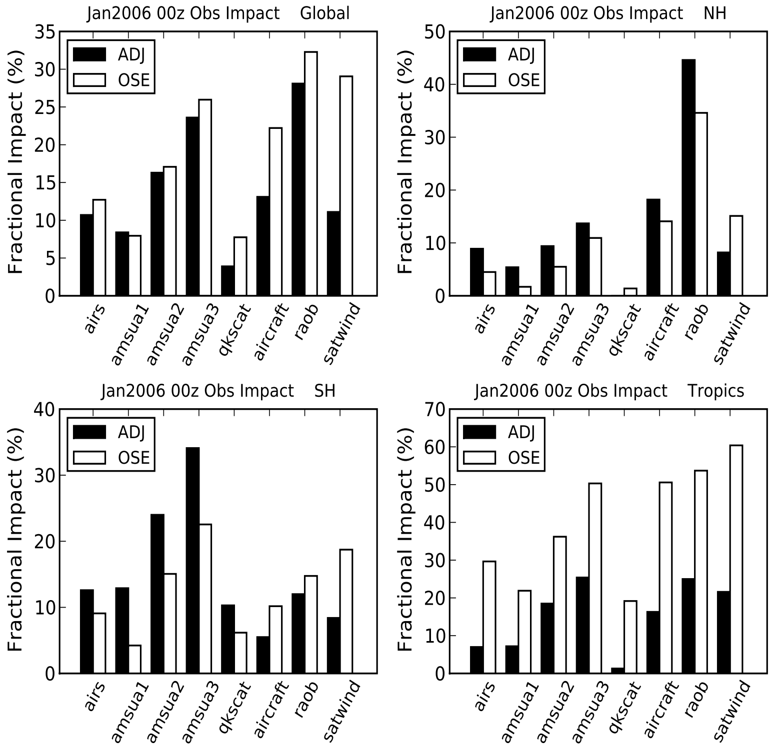


*Figure 5: Adjoint- and OSE-based fractional impacts of various observing systems on the change in 24-h forecast error over the globe (upper left), NH (upper right), SH (lower left) and tropics (lower right) during January 2006 (Gelaro and Zhu 2009).*

## 4 Comparison of adjoint-based observation impact with OSEs

The impact of observations on (1) can also be assessed using OSEs, by computing differences in $e$ between a control forecast including all observation types assimilated routinely and forecasts in which selected observations have been removed from the data assimilation system. Gelaro and Zhu (2009) conduced a detailed comparison of adjoint-based observation impacts with those obtained from OSEs using a version of the GEOS-5 forecast system. Examples of their results are reproduced here.

To compare the methods, these authors defined for each approach a measure of the fractional impact of an observing system $j$ to the total error reduction obtained from the complete set observations assimilated. For the adjoint method, the fractional impact is defined as

$$F_j(\mathrm{ADJ}) = \delta e_j / \delta e\,, \tag{8}$$

where $\delta e_j$ is the partial sum of $\delta e$ corresponding to observing system $j$. For the OSEs, the fractional impact is defined as

$$F_j(\mathrm{OSE}) = (e_{j*} - e_{ctl})/e_{ctl}\,, \tag{9}$$

where $e_{j*}$ is the error measure of the 24-h forecast from the analyzed state *without* observing system $j$ and $e_{ctl}$ is the error measure of the 24-h forecast control forecast including all observations.

Fig. 5 compares the values of $F_j(\mathrm{ADJ})$ and $F_j(\mathrm{OSE})$ for January 2006 for eight observing systems tested in the OSEs. The observing systems are identified along the abscissa; the suffixes 1, 2 and 3 for AMSU-A denote impacts of one, two and three AMSU-A instruments. Over the globe and extratropics, we see fairly

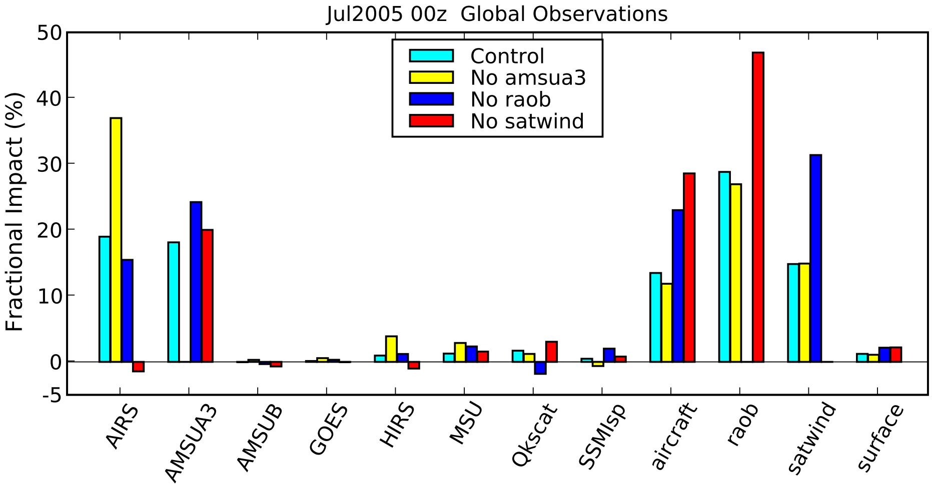


*Figure 6: Adjoint-based fractional impacts of various observing systems on the change in 24-h forecast error during July 2005 for different OSEs. Results include only contributions from observations in the tropics to the reduction in global forecast error (Gelaro and Zhu 2009).*

good quantitative agreement between the two measures for most observing systems, with the exception of the satellite winds globally. In the NH there is good agreement for all observing systems. In the SH we see somewhat larger impacts for AMSU-A in the adjoint results, as well as the larger impact of satellite winds in the OSE results seen globally.

In the tropics, there is greater disagreement overall between adjoint and OSE results. Values of $F_j(\mathrm{OSE})$ are much larger than those of $F_j(\mathrm{ADJ})$ for all observing systems, with the former exceeding 50% for several observing systems. In the adjoint results, it is impossible to have such large fractional contributions from several observing systems simultaneously since the sum fractional impact for all observing systems must equal one. There is no such constraint on the fractional impacts in the OSEs, which are based on a series of separate experiments. Nonetheless, the relative magnitudes of the various observing system contributions are consistent in the two sets of results. This can be seen more clearly by normalizing the results in the tropics for each method (not shown).

The *combined* use of OSEs and adjoints provides insights into how (changes in) the mix of observations in a data assimilation system affects their impacts. This can be measured by applying the adjoint method to the perturbed OSE members and comparing the impacts of the remaining observing systems with those in the control experiment. Fig. 6 compares the fractional impacts in the control experiment with those in the *no amsua3*, *no raob* and *no satwind* experiments during July 2005. In this case, we show contributions from observations in the tropics to the reduction of the global error norm. There are large variations in the impacts of several observing systems. Removal of the satellite winds increases the impact of rawinsondes by more than two thirds compared with the control, from 28% to 47%. There is a reciprocal response in the impact of satellite winds to the removal of rawinsondes, which more than doubles with respect to the control experiment, increasing from 15% to more than 30%.

The response of AIRS is more complex. The removal of AMSU-A radiances nearly doubles the fractional impact of AIRS from 19% to 37% with respect to the control. In sharp contrast to this, however, the removal of the satellite winds results in AIRS having an overall detrimental impact on the forecast. This results suggests that, in the absence (or substantial reduction) of direct observations of the wind, the wind increments induced by AIRS through the balance relationship alone are detrimental at these latitudes.

## 5 Conclusions

Adjoint-based estimates of observation impact have become increasingly popular as an alternative or complement to traditional observing system experiments (OSEs). The adjoint technique is currently used at several forecast centers for experimentation or routine monitoring of the observing system. Interest in the adjoint method has motivated an inter-comparison project between centers to directly compare observation impacts in different operational forecast systems. Initial results comparing observation impacts in the US Navy NOGAPS and NASA GEOS-5 forecast systems were presented. Results so far reveal overall consistency between the impacts of most major observing systems in the NASA and Navy systems, despite basic differences in the respective analysis algorithms, radiative transfer models and observation counts for some observation types.

For linear analysis problems, observation impact is closely related to (is an extension of) observation sensitivity. For nonlinear analysis problems, such as those solved using an incremental variational data assimilation scheme, computation of observation impact is more complicated. A simplified treatment of the outer loop contributions is possible, however, providing useful estimates of observation impact for these systems.

Comparisons so far between observation impacts derived from OSEs and the adjoint method reveal overall consistent estimates of the “importance” of most of the major observing systems, despite fundamental differences in their underlying assumptions and methodologies. Information gleaned from OSEs and adjoints should be viewed as complementary since both address relevant questions about how observations influence the quality of weather forecasts. It is important to keep in mind that the adjoint measures the impact of observations in each analysis cycle separately and against the control background containing all previous information, while the OSEs measure the impact of removing observational information from both the background and analysis in a cumulative manner. This distinction can be significant, especially if an observing system contributes disproportionately to the quality of the analysis and subsequent background state.

The *combined* use of OSEs and adjoints provides insights into how (changes in) the mix of observations in a data assimilation system affects their impacts. Information about these dependencies may be useful for making intelligent data selection decisions and possibly identifying needs for future observation types.

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