

Interactive comment on “Development of the adjoint of GEOS-Chem” by D. K. Henze and J. H. Seinfeld

D. K. Henze and J. H. Seinfeld

Received and published: 4 February 2007

Response to reviewer #1

1. *line 100 after Equation (1), “... species observations mapped to the model domain space ...”: The more common approach would be mapping variables from model space to observation space. It is sometimes impossible to do it the other way. Please comment on this.*

For something like satellite observations, it is definitely preferable to map predictions to the observation space. On the other hand, for aerosol filter samples (collected over a period of several hours), the mapping process is somewhat of a combination, as measurements from multiple sources get averaged over the model grid, while the model predictions are averaged over the filter collection pe-

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

Discussion Paper

riod. Though the actual process will be application specific, for consistency, we have changed the text to read “ c is the vector of species concentrations mapped to the observation space, c_{obs} is the vector of species observations.”

2. *line 197, “We use $\delta\sigma=0.1-0.01 \dots$ ”: The value of “ $\delta\sigma=0.1-0.01$ ” used to calculate the derivatives seems too big. Please explain why such a range is chosen. In addition, the derivatives calculated using $\sigma=0.1$ would be significantly shifted from the adjoint counter part. That is, the derivative by the one-sided finite difference is indeed at $\sigma + 0.05$ while the adjoint gives the derivative at σ .*

We have attempted to clarify issues related to calculation of finite difference sensitivities, Λ , see the first paragraphs of Sect. 3. For testing adjoint code for particular processes, the manner in which Λ is calculated can make an appreciable difference. For discrete adjoints of nonlinear processes, agreement between λ and Λ is best when $\delta\sigma$ is small, shown now in Fig. (2), while for comparisons including advection, using larger perturbations can minimize discrepancies owing to discontinuities of the discrete advection routine, see Fig. (4). Also, the trade off between truncation error ($\sim \delta\sigma$) and roundoff error ($\sim \frac{1}{\delta\sigma}$) must be balanced. Values smaller than $\delta\sigma = 0.01$ do not always induce a large enough change in the cost function to rise above the roundoff error, particularly when considering effects of a single parameter on a global burden, and considering that data are checkpointed only to single precision. However, for tests with the complete model, using one-sided vs two-sided perturbations, with $\delta\sigma=0.1-0.01$, was not found to have an appreciable effect on the overall correlation between λ and Λ ; hence, the more approximate one-sided finite difference approximation was used in the full model tests (Sect. 3.5) for efficiency.

3. *line 212, “... though these methods are used mostly in other fields”: Does this imply that the methods cannot be applied here?*

No. Regardless, the section containing this comment has been replaced by more

pertinent material.

4. *line 243, “hence, λ has units of s^{-1} ”: Please differentiate adjoint state variables and the adjoint derivatives. The units appear to be s rather than s^{-1} .*

Indeed, the units should be s . These results are now presented as a plot of the dimensionless ratio $\lambda_{ENO_x} / \Lambda_{ENO_x}$, see comment 6. The adjoint variable has been given distinctive subscripts.

5. *line 258 and Table 1: Please provide references for full names of the species.*

While this table has been replaced by Fig. 2, a reference for full species names is now given where such abbreviations arise in Appendix A.

6. *line 263, “the ratio $\lambda_{ENO_x} / \Lambda_{ENO_x}$ becomes 1.07 and 0.94”: Those numbers are not close enough to 1. It might be due to the way the finite difference was carried out, as mentioned previously. If it cannot be improved, please elaborate possible causes.*

The reviewer is correct in that the method of the finite difference calculation was partly contributing to ratios deviating from unity. Using a smaller perturbation leads to improved agreement for these box model tests, with ratios deviating by only a few percent from unity. In order to clarify, Table 1 has been replaced by Fig. 2, which explicitly shows how the finite difference calculations affect the ratio $\lambda_{ENO_x} / \Lambda_{ENO_x}$. Additionally, using a fixed internal time step gives increasingly precise results.

7. *lines 583-585, “... however, this would risk over-optimization ...”: What is over-optimization? The possible oscillatory behavior is not due to more iterations. It could indicate that the problem does not have a unique solution. Please clarify.*

The smoothing properties of the transport operator admit solutions with components that lie in the null space of the forward model. Such components of the

[Full Screen / Esc](#)[Printer-friendly Version](#)[Interactive Discussion](#)[Discussion Paper](#)

solution are necessarily the high frequency ones, hence optimization when the cost function is not adequately constrained can lead to oscillatory behavior. Multiple solutions can also arise if insufficient observations are available to constrain the inversion. The remedy for both problems is to avoid overly minimizing the predictive error term of the cost function, either by formally including additional constraints (regularization) or, more informally, by halting the optimization before the solution begins to exhibit such features. The text has been changed to read, “Further iterations might be justified; however, care must be taken to avoid overly minimizing the predictive error component of the cost function at the sake of generating noisy solutions.”

8. *lines 661-662: Please define RTOL and ATOL.*

RTOL and ATOL are the relative and absolute error tolerance levels, respectively. These terms are now defined within the text.

9. *Figures 1-2: It is better to present the distribution of $\lambda_{ENO_x}/\Lambda_{ENO_x}$ in place of λ_{ENO_x} or Λ_{ENO_x} for the purpose of validation.*

The reviewer makes an excellent suggestion. We now show a map of only the adjoint sensitivities, but also include a scatter plot of adjoint vs finite difference sensitivities. As lack of transport leads to unrealistically extreme concentrations, emissions are reduced by an order of magnitude for these tests to prevent the chemical systems from becoming too stiff.

10. *Figure 4: Consider using log scales for some of the plots.*

This was considered, but many of the values shown are negative. Rather than transform the gradients, it was deemed preferable to include expanded view plots on linear scales to magnify clusters of points when necessary.

Technical corrections suggested by the reviewer have been fixed.

Interactive comment on Atmos. Chem. Phys. Discuss., 6, 10591, 2006.

ACPD

6, S6632–S6636, 2007

Interactive
Comment

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

Discussion Paper

S6636

EGU