Geosci. Model Dev. Discuss., 6, C2642–C2645, 2014
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Geoscientific Model Development Discussions Open Access

Interactive comment on "Development of a variational flux inversion system (INVICAT v1.0) within the TOMCAT chemical transport model" *by* C. Wilson et al.

Anonymous Referee #1

Received and published: 23 February 2014

1 Overview

The manuscript by Wilson et al., "Development of a variational flux inversion system (INVICAT v1.0) within the TOMCAT chemical transport model" presents a new 4D-Var tool for inverse modeling of atmospheric tracers, such as CO_2 or CH_4. The authors present a clear overview of the utilities of this tool, followed by details of how it was constructed, and concluding with validation tests of the adjoint model gradients as well as a simple toy inversion. Overall the manuscript is clear and well written. My only overall suggestion is that in some places the text can be thinned a bit. Below are some specific suggestions to help clarify this and a few other aspects. This manuscript will

be suitable for publication after minor revision.

2 Specific comments

- The authors might consider a different / revised title. Currently it implies that INVICAT is contained within TOMCAT, but rather the TOMCAT model would be contained within INVICAT, which comprises TOMCAT, ATOMCAT, and M1QN3.
- 7120.20: similar that → similar to that
- 7120.28: possible → is reasonable? Because it's always possible to change them quite a bit, it just might not be reasonable.
- 7124.22: modelling explained → modelling are explained
- 7125:8: The reference here seems quite outdated. There are any number of more recent papers analyzing the performance of L-BFGS in the context of modern 4D-Var problems; I would suggest including something along these lines.
- 7125.21: At this point in the manuscript I wonder what the difference is between M' and M, both of which seem to be the linearized forward model. Is it possible to unify the notation?
- The authors discuss checkpointing a bit, but typically this is only necessary for nonlinear processes. Tracer transport is, on paper, linear. So can they explain what is necessary to checkpoint? Is this because of the nonlinearities in the advection algorithm?
- 7126.10: Strictly speaking, it's not correct to say that the adjoint calculates the sensitivity of c. Rather, it calculates the sensitivity of scalar metrics of c, such as J. Calculating the sensitivity of c would be the complete Jacobian, which is

computationally prohibitive. Same issue regarding the text on line 24 of page 7120.

- 7126.20: The authors justify the discrete approach for taking the adjoint of their advection scheme though Sirkes and Tziperman (1997). However, the work of Gou and Sandu (Atmospheric Env., 2011) provides a more relevant example, and, more importantly, they show that the discrete adjoint can actually lead to *worse* performance than the continuos adjoint for 4D-Var applications with CTMs. Granted, the outcome is likely dependent upon the actual advection scheme employed. Since the authors don't appear to be using either the scheme from Sirkes and Tziperman (leap frog) or that studied in Gou and Sandu (piece-wise parabolic), they may need to think more carefully about the justification for their particular model.
- 7129.6: 2001) and → 2001), and
- Regarding the Lagrange equality test, I have two concerns. First, this check can potentially overlook fortuitous cancelation of errors if the variables being tested are vectors, as is implied by the notation in the manuscript. A more stringent, albeit costly, test is to check individual variables. Second, in my experience a significant challenge in developing an adjoint is not the creation of adjoints of individual subroutines, but rather the "glueing" back all of the individual adjoint subroutines together in correct way. Thus I'm a bit concerned that the authors only test their subroutines for a single iteration (7134.5). Can they test over longer periods? Can they compare individual sensitivities to brute force (finite difference) sensitivities?
- The reciprocity test is a nice way of checking the transport adjoint validity.
- The inverse modeling test is perhaps overly simple, mainly in that it doesn't appear that any random error was ascribed to the observations. Most of the issues

related to inverse modeling won't become apparent until noise is included in the observed data, so the results shown here will not likely be representative of the performance achieved in any real application.

- 7120.19: It might be good to explain what the differences are here.
- 7121.5-9: This is a bit strongly worded, suggest rephrase. I recognize that the availability of satellite data has driven the method to advance a lot in atmospheric chemistry the past decade, but the adjoint-based variational inverse method itself has been used decades earlier (e.g., nuclear reactor design in the 1940's) in other fields.
- The material starting on the last line of 7123 through line 9 of 7124 feels redundant and unnecessary. The meaning of the cost function has already been explained. The utility of defining the cost function terms separately is not apparent.
- 7124.25 – 7125.9: Since the details of the optimization are presented later, it doesn't seem necessary to describe the process qualitatively here.
- 7126.23: accurate in comparison → consistent with
- 7133.3: The sentence "These tests . . . " seems somewhat expendable.
- 7136.12: If I'm not mistaken, this uses the BFGS algorithm, so that should be mentioned specifically with appropriate references.
- 7139.16: Presenting this as an equation with no equality is a bit odd.
- Appendix A: given the vast body of literature using adjoint models for gradient-based optimization, it doesn't seem that this section is necessary.

Interactive comment on Geosci. Model Dev. Discuss., 6, 7117, 2013.