Geoscientific
Model Development
Discussions

Interactive comment on "A generalized tagging method" *by* V. Grewe

V. Grewe

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I like to thank the reviewer for the helpful comments. Below, reply to all comments (comments are in bold) in more detail. The comments show basically two issues:

- The methodology was not compared to other approaches in detail. As a consequence, the reviewer didn't fully realize that this diagnostics is actually new, though based on previous work from chemical diagnostics (chemical tagging) and here "just" generalizes this approach, as correctly stated by the other reviewer. Therefore a brief discussion is added in the introduction and additionally a section is included, which intercompares tagging with other methods for a very simple parametric system. An overview is given in a table (see attachment- table 2). This should give a better basis for the understanding of the tagging diagnostics. Just to avoid misunderstandings: Tagging is not solving all problems,

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but it is a very useful addition to existing diagnostics and moreover, in non-linear systems, it is the only method, as far as I know, which aims at calculating contributions of a source to a quantity in a deterministic manner for every time-step and location.

- The mathematical notation was not clear enough. I included a table (see attachment - table 1), which gives a detailed overview on the notation, clarifying this issue.

A more generalized formulation for making attribution calculations with a numerical model for chemistry and climate is presented. It is a useful contribution, but needs to be made more accessible by recognizing the parallels with other methods and explaining some aspects of the mathematics. As far as I can see this approach looks at the parts of the continuity (tendency) equation that can be partitioned among different sourced tracers and then generates a tendency in other tracers based on the Jacobian and a decomposition of net P-L terms to deal with the non-linear (non-additive) nature of parsing the total tendency into its components.

Reply: Basically correct.

Tagging is just one approach to following the consequences of a specific perturbation and then attributing down-link consequences (ozone depletion, climate change). The most straightforward way to do this is to perform both control and perturbation numerical calculations and then to difference them. These are described as sensitivity/ perturbation experiments here. The obvious issue with perturbation calculations is that they are effectively a linearization of the system about the current state, and do not apply as one drops all anthropogenic emissions or other sources and the system shifts to a very different state with different sensitivities.

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Reply: Fully agreed and in agreement with e.g. Grewe et al., 2010.

The manuscript derides sensitivity calculations (with the case of tropospheric ozone production) in that a NOx saturated regime is insensitive to added NOx. But that is true: Perturbations to NOx have little impact, but if one were to eliminate all the NOx and then add a perturbation, the NOx would generate much more ozone.

Reply: "derides?". I have no intention to deride previous methods. I think the method is fine for specific purposes, but not all purposes. The introduction reads: "provides a valuable information on the sensitivity ...". This is not deriding the method. I went through the manuscript and didn't see where I caused this interpretation. I am happy to revise any statement, which may lead to such an unintendet position.

I basically agree on the chemistry, an addition of NOx does not result in an addition of ozone in a saturated regime. However, the chemistry is changing, the specific ozone production, i.e. the ozone production oer NOx molecule decreases. Hence, the addition of NOx actually changes the chemistry and changes the contribution of individual NOx sources to ozone, without changing its sum.

This is a problem with any non-linear system, and it cannot be fixed with tagging or any other approach as all of them must make arbitrary decisions in framing the question. Thus, the example here has no "correct" answer.

Reply: Here, I disagree. Let's take a grid cell in which 40 NOx molecules produced 80 ozone molecules by non-linear chemistry (meaning that 42 NOx molecules would have produced, e.g., 79 ozone molecules). Then we can state that every NOx molecule has produced two ozone molecules. The chemisty is not distinguishing between the origin of the NOx molecules, whether they ae emitted by road traffic or lightning. For the chemistry they are equally important at that time and location. And hence if there were 10 NOx molecules from lightning and 30 from road traffic, then lightning has produced 20 ozone molecules and road traffic produced 60 ozone molecules.

Moreover, if I follow the derivations here correctly, then the ultimate equation (10) is really no different than the sensitivity runs. Effectively the tendency (F) is merely partitioned among the various tagged tracers using the Jacobian, which is only a linearization about the current state. The perturbation / sensitivity runs implicitly use this same linearization.

Reply: No, there is a big difference, although both approaches might look similar. The perturbation approachs basically is a derivative of a quantity x with respect to the source in question. For example the derivative of ozone concentration with respect to road traffic NOx emissions. Tagging on the other side differentiates individual production and loss terms with respect to the quantities in question, and not to the to the sources, e.g. the derivative of the production of ozone with respect to the concentration of NO and HO2. Two very different things, which have been shown to potentially differ by orders of magnitude and even in sign for even simple non-linear systems (Grewe et al., 2010) and by a factor of 5 for road traffic simulations (Grewe et al., 2012). This issue will be discussed in more detail in the newly introduced intercomparison section based on a simple non-linear system, where this differences can be calculated analytically.

The singularity issue is interesting, but seems to be just a zero-dividedby- zero issue?

Reply: Yes it is a division by zero problem. If, e.g., the sensitivities are -5 and +5 then the specific sensitivities would be -5/0 and +5/0. And hence is a principal limitation of this "ansatz".

The heating rate section has analogies with the UV radiative coupling of the N2O-O3 system (Prather, Science 1998) in which the coupling is across all levels. It becomes an (n-species x m-levels)-squared problem. While this worked in a 1-D diffusion model, I doubt that the tagging across all levels is practical in a 3-D model as the matrices described here would become unmanageable.

Reply: Indeed, from an computational aspect, tagging requires a lot of memory, but

only few computing time. We are currently running a system with 10 species and 10 categories of all levels (which are 41). This works. Since the work of Prather (1998) differs from the tagging approach, this might cause the irritation?

This approach needs a serious re-think. If published, the author should fix some of the following: 3312/15-3313/13 I think differences between this method and the perturbation method are not that great. The answers should be the same unless you make arbitrary decisions about the non-linearity. 3313/7-11 This is the problem with tagging. The simple perturbation calculation includes all of these automatically.

Reply: No, I think previous studies have clearly shown that the two approaches are different in nature, answer different questions, and should not be interchanged. though, I think a combination of both methods will actually provide a much better understanding of simulated changes (see previous comment and Grewe et al., 2012). Since this is every now and then a point of discussion, I added an example in a new section, which actually shows this in a simple way.

3313/22 "ansatz" is not a common English word, try another.

Reply: "Ansatz" is a mathematical term, which describes exatly what I would like to express here, namely the mathematical description of a word problem. (See e.g. http://encyclopedia.thefreedictionary.com/Ansatz.)

3315/ From here on out it is not clear what quantities are vectors, matrices, scalars . can you help clear this up? Equation (10) for example . the multiplier of F(x) is a scalar? Also, the GRAD F notation appears in (10) without definition.

Reply: The revised version will include an overview table, explaining all variables. E.g. $F(x)$ was defined as a vector (just above equation (1)). Nabla F = gradient of F with respect to x, where x is a vector. I assumed this is standard mathematics, but I agree an explicit definition is definitely helpful and avoids misunderstandings.

3321/12 Missing a word: which allows to

Reply: corrected

3321/19 "ansatz" again

Reply: see above

Interactive comment on Geosci. Model Dev. Discuss., 5, 3311, 2012.

Interactive
Comment

Table 1. Overview on used variables. The time dependency "(t)" is omitted occasionally For simplicity reasons. E.g. $\boldsymbol{x}(t)$ becomes $\boldsymbol{x}$.

Variable	Description	Comment
i	Index for n state variables x_i	$i = 1, \ldots, n$
j	Index for m sources contributing to state variables x_i	$j = 1, \ldots, m$
$x_i(t)$	Time dependent state variable	e.g. temperature or ozone concentration
$x_i^j(t)$	Time dependent contribution of source j to state variable x_i	$\sum_{j=1}^m x_i^j = x_i$
$\boldsymbol{x}(t) = \begin{pmatrix} x_1(t) \\ \vdots \\ x_n(t) \end{pmatrix}$	State variables	
$\boldsymbol{x}^j(t) = \begin{pmatrix} x_1^j(t) \\ \vdots \\ x_n^j(t) \end{pmatrix}$	Time dependent contribution of source j to x	
$X(t) = \begin{pmatrix} x_1^1(t) & \ldots & x_1^m(t) \\ \vdots & & \vdots \\ x_n^1(t) & \ldots & x_n^m(t) \end{pmatrix}$	Contribution matrix	$X \times \mathbb{1} = \boldsymbol{x}$
$\boldsymbol{P}(t) = \begin{pmatrix} P_1(t) \\ \vdots \\ P_n(t) \end{pmatrix}$	Time dependent external forcings	
$\boldsymbol{F}(\boldsymbol{x}) = \begin{pmatrix} F_1(x_1, \ldots, x_n) \\ \vdots \\ F_n(x_1, \ldots, x_n) \end{pmatrix}$	Forcings depending on state variables	$\frac{\partial}{\partial t} \boldsymbol{x}(t) = \boldsymbol{P}(t) + \boldsymbol{F}(x)$
P_i^j	Contribution of source j to the external forcing P_i	$\sum_{j=1}^m P_i^j = P_i$
F_i^j	Contribution of source j to forcing F_i	$F_i^j = \frac{Q_i^j}{T_i} F_i$ (see below); $\sum_{j=1}^m F_i^j = F_i$ in vector notation :
$Q_i^j = (x_i^1, \ldots, x_i^m) \begin{pmatrix} \frac{\partial F_i(\boldsymbol{x})}{x_1^j} \\ \vdots \\ \frac{\partial F_i(\boldsymbol{x})}{x_i^m} \end{pmatrix}$	Impact of source j on F_i	$Q_i^j = \boldsymbol{x}^{j^\mathrm{T}} \frac{\partial F_i(\boldsymbol{x})}{\partial x}$ $= \boldsymbol{x}^{j^\mathrm{T}} \left(\frac{\partial F_i(\boldsymbol{x})}{\partial x} \frac{\partial x}{\partial x^j} \right) = \boldsymbol{x}^{j^\mathrm{T}} \frac{\partial F_i(\boldsymbol{x})}{\partial x}$ $= \boldsymbol{x}^{j^\mathrm{T}} \nabla F_i(\boldsymbol{x})$
$\nabla F_i(\boldsymbol{x}) = \begin{pmatrix} \frac{\partial F_i(\boldsymbol{x})}{\partial x_1} \\ \vdots \\ \frac{\partial F_i(\boldsymbol{x})}{\partial x_n} \end{pmatrix}$	Gradient of F_i	
$T_i = \sum_{j=1}^m Q_i^j$	Total impact of all sources on F_i	
$\frac{Q_i^j}{T_i}$	Contribution of category j to the total impact	$\sum_{j=1}^m \frac{Q_i^j}{T_i} = 1$

Table 2. Overview on the characteristics of the non-linear system $\dot{x} = P - x^\alpha$. See Sec. 5 for details.

Description	Variable	Result
Steady-state solution	x^s	$= P^{\frac{1}{\alpha}} = P \tau_x$
Lifetime of x	τ_x	$= P^{\frac{1-\alpha}{\alpha}}$
Lifetime of a perturbation y to x^s	τ_y	$= \alpha P^{\frac{1-\alpha}{\alpha}} = \alpha \tau_x$
Steady-state solution of tagged quantity	${}^t x_i^s$	$= P_i P^{\frac{1-\alpha}{\alpha}} = P_i \tau_x$
Contribution calculated with perturbation approach	${}^p x_i^s$	$= \frac{1}{\alpha} P_i P^{\frac{1-\alpha}{\alpha}} = P_i \tau_y$

Fig. 1. Additional tables