Automatic differentiation in the analysis of strategies for mitigation of global change

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EXTENDED ABSTRACT

The likelihood of major changes in the global climate, caused by continuing emissions of greenhouse gases has led to numerous proposals for reductions in emissions, with the Kyoto Protocol being only a small and incomplete step. As well as the usual problems associated with decision-making under uncertainty, measures for mitigation of global warming involve a cascade of long time-scales associated with energy investments, carbon-cycle response and climate response.

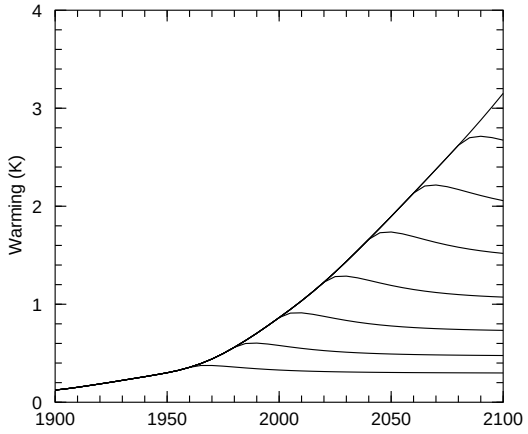

Figure 1. Temperature increase from CO_2, assuming emissions as for Figure 1, attributing warming to successive 20-year emission periods.

Figure 1 illustrates some of the long time-scales involved. The bands represent the temperature given emissions that go to zero after the respective cutoff times. One feature is that even if emissions go to zero, temperatures continue to increase for some time. This effect is termed 'committed warming'. It occurs because even though CO_2 starts to decline after emissions cease, the ocean has not come to equilibrium.

In analysing such a situation, modelling activities have to include actions such as calibration, data assimilation and sensitivity analysis. Automatic differentiation provides an important tool for transforming computer models into a modelling system capable of performing these various tasks.

This talk describes the use of automatic differentiation based on C++ classes and operator overloading. This allows derivatives to be calculated with minimal changes to the underlying model.

One important class of sensitivity analysis is associated with the so-called Brazilian Proposal. This was introduced during the negotiations leading to the Kyoto Protocol and envisages targets for emission reductions being set on the basis of nations' relative responsibility for global warming. A differential formalism is one of the approaches that has been considered for attribution of non-linear effects. Examples are presented.

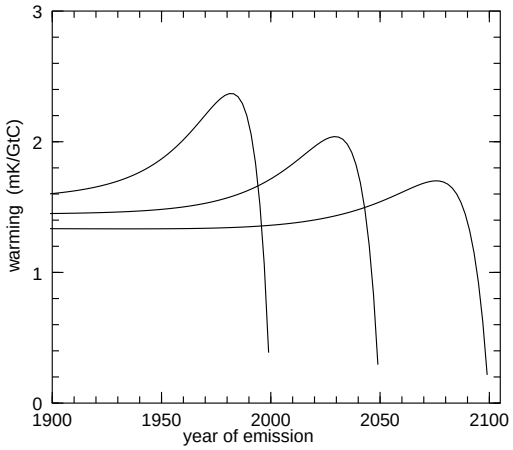

Figure 2. Curves $S_{2000}(t)$, $S_{2050}(t)$ and $S_{2100}(t)$ giving the warming (in milliKelvin per gigatonne of carbon) in the years 2000, 2050 and 2100 due to CO_2 emissions over time.

Higher-order derivatives can then be used to determine the extent to which such differential responsibilities are sensitive to uncertainties in the representation of global change.

1. INTRODUCTION

Radiatively active gases such as carbon dioxide (CO_2) and methane (CH_4), commonly called greenhouse gases, have been increasing in the atmosphere over the last few centuries of increasingly rapid industrialisation. It is now virtually certain that this has led to global warming and will continue to do so. Since the most important anthropogenic greenhouse gas is CO_2, an inevitable product of using fossil energy sources, mitigation actions will be extremely difficult.

A further difficulty in achieving effective action comes from the long time-scales involved. While some CO_2 is removed from the atmosphere quite rapidly, about 15% of any input remains in the atmosphere for time-scales of millennia or more. Similarly, the climate system responds slowly to changes in greenhouse gas forcing, with the oceans and ice-sheets taking many centuries to come into thermal equilibrium.

These issues are illustrated in Figures 1 and 3. These consider cases where CO_2 emissions follow historical values succeeded by 'business-as-usual' projections, up to a time t and are then zero thereafter. Performing this calculation for a succession of cutoff times partitions the concentration into bands that can be attributed to successive 20-year time intervals. In Figure 3, the lowest band represents concentrations from pre-1960 emissions, the next band, emissions from 1960 to 1980 and so on.

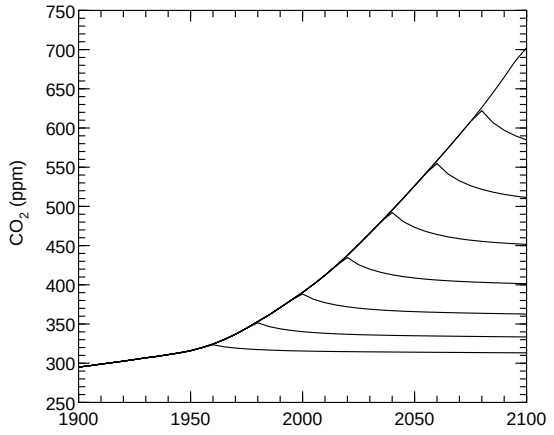

Figure 3. Atmospheric CO_2, given historical emissions and business-as-usual (IS92a) projections, partitioned according to emissions in 20-year periods.

These calculations can be extended to temperature as is done in Figure 1. Again the bands represent the temperature given emissions that go to zero after the respective cutoff times. One feature is the 'committed warming' , also termed 'unrealised warming', (e.g. Wetherald *et al.*, 2001) where temperatures continue to increase for some time, even though CO_2 starts to decline after emissions cease. This is because the ocean has not come to equilibrium.

A number of policy measures have been developed to address the risks from climate change. The Framework Convention on Climate Change (FCCC) commits signatories to address the issues. Under the FCCC, the Kyoto Protocol sets specific emission targets for the developed nations for the first commitment period (2008–2012). Longer-term approaches have been discussed, both during the Kyoto Protocol negotiations and in the wider policy discourse. One general framework, termed 'Contraction and Convergence' envisages moving towards uniform *per capita* emissions (of around 1 to 2 tonnes of carbon per person year) towards the end of the 21st century. Other frameworks included sector-based targets (Phylipsen *et al.*, 1998). This approach underlies internal target-setting within the EU 'bubble' target. A proposal by McKibbin and Wilcoxen (2002) is more concerned with the economic aspects of implementing targets, rather than the specific form of target. The present paper analyses aspects of an approach, proposed by Brazil during the Kyoto Protocol negotiations, for emission reduction targets to be set in proportion to each nation's historical responsibility for global warming.

Although the fact of anthropogenic global warming is scientifically well-established, significant quantitative uncertainty remains. While the need to make complex decisions under significant uncertainty is hardly unique to the climate change issue, some of the important uncertainties can be quantified. Quantification of uncertainty is also important in the face of politicised exaggerations of the uncertainties.

2. MODELLING

Modelling of global change involves models of many different types. A useful way of categorising models is in terms of the spectrum described by Karplus (1977). This describes models as running from black-box models or a 'curve-fitting' type through to 'white-box' models constructed, generally as deterministic models, in a mechanistic form based on underlying scientific principles. Enting (1987) used this model spectrum framework to characterise carbon cycle models as running from curve-fitting, through the use of a constant airborne fraction, representations in terms of response functions, highly-lumped 'box-models', through to models with mechanistic representations of oceanic and biological systems. Similarly, climate models can be thought of in terms

of a spectrum from curve-fitting through response functions, energy-balance models, general-circulation models and earth system models allowing feedbacks between various components.

The modelling for the Brazilian proposal specified response functions as the default case, for both trace gases and climate response.

The components that we consider, using relations from Enting and Trudinger (2002), are: the relation between emissions and concentration, the relation between concentrations and radiative forcing and the relation between radiative forcing and warming.

When response functions are expressed as sums of exponentials, the response function form is readily converted to an equivalent set of first-order differential equations (e.g. Wigley, 1991).

For a model expressed as N coupled differential equations:

$$\frac{d}{dt}x_j = g_j(\{x_k\}, \alpha, t) \qquad \text{for } j = 1, N \qquad (1)$$

we can define sensitivities as

$$y_j = \frac{\partial}{\partial \alpha} x_j \qquad \text{for } j = 1, N \qquad (2)$$

to give what is known as 'the tangent linear model':

$$\frac{d}{dt}y_m = \frac{\partial}{\partial \alpha} g_m(\{x_k\}, \alpha, t) + \sum_n \frac{\partial}{\partial x_n} g_m(\{x_k\}, \alpha, t) y_n \qquad (3)$$

An important characteristic of the tangent linear model, is that it is indeed linear in the $y_n(t)$ given the basic model solution $x_m(t)$ for all m. This linearity implies the existence of an adjoint model (the model whose Green's function is the adjoint of the Green's function for the tangent linear model) which gives the time evolution of quantities of the form $\frac{\partial \phi}{\partial x_m}$. Efficient implementation of such adjoint models (corresponding to sparse matrix factorisations of successive application of the rules of differentiation) requires that the adjoint model be integrated backwards in time. This requires storage of the functions $x_n(t)$, unlike equation (3) where the $x_n(t)$ can be evaluated by parallel integration of (1) and (3). Actual construction of programs for tangent linear and adjoint models is often undertaken using automatic differentiation.

3. AUTOMATIC DIFFERENTIATION

While the primary function of many computer models is integration – projecting into the future – a number of the operations involved in analysing models actually involve differentiation. These include: initialisation, calibration, sensitivity studies, and data assimilation.

While the requisite derivatives can often be calculated with sufficient accuracy by finite differencing, it is often desirable to have a program that calculates these derivatives directly. Such a capability helps turn a 'computer model' into a computer 'model analysis system' — this term is preferable (being less ambiguous) to the term 'modelling system' proposed by Kaminski *et al.* (2003).

Automatic differentiation provides an important tool for transforming computer models into a model analysis system for performing these various tasks.

There are several ways of doing this:

A The same effect can be produced by hand-coding a program to calculate the derivatives — this is laborious, error-prone and needs to be repeated each time the model changes.

B In many cases, symbolic algebra systems such as Mathematica can be programmed to produce derivatives by adding a single command to the program – producing adjoint models in this way would seem problematic.

C Tangent/adjoint compilers are tools that analyse the source code for a model and produce code that implements the tangent-linear or adjoint models.

D Rather than analysing the program directly, operator overloading of steps in a model can be used to produce a 'script' that can be analysed to produce code for the derivatives — projects to implement this approach are ADOL-F and ADOL-C (using Fortran and C++ respectively).

E Another approach, described below, is to use the operator overloading capabilities directly – this is straightforward for the tangent-linear-model, but the application to adjoint modelling is more difficult and more restricted in scope.

Operator overloading involves replacing a real scalar variable x, represented as type `double`, with a composite variable $\tilde{x}$ represented in the program as type `Xvar`. The composite variable represents both the value x and its derivatives with respect to J model quantities, α_J as:

$$\begin{cases} \tilde{x}_0 = x \\ \tilde{x}_n = \frac{\partial}{\partial \alpha_n} x \qquad \text{for } n = 1, J \end{cases}$$

Overload operators are defined for such variables as

implementations of $\tilde{c} = \tilde{a} * \tilde{b}$, representing:

$$\begin{cases} \tilde{c}_0 = \tilde{a}_0 * \tilde{b}_0 \\ \tilde{c}_n = \tilde{a}_0 * \tilde{b}_n + \tilde{a}_n * \tilde{b}_0 \end{cases}$$

and overloaded functions are defined, with $\tilde{c} = f(\tilde{a})$ representing:

$$\begin{cases} \tilde{c}_0 = f(\tilde{a}_0) \\ \tilde{c}_n = f'(\tilde{a}_0) * \tilde{a}_n \end{cases}$$

where $f'(.)$ denotes the derivative of $f(.)$

The following code fragment shows part of the C++ class definition that implements this operator overloading:

```
class Xvar{
public :
static const int ns = _NUMDERIVS+1;
double xs[_NUMDERIVS+1];
Xvar operator*(Xvar);
...
};
```

```
Xvar Xvar::operator*(Xvar b){ Xvar
c;
for (int i=1; i < ns; i++) c.xs[i]
= xs[i]*b.xs[0]+xs[0]*b.xs[i];
c.xs[0] = xs[0]*b.xs[0];
return c;} ;
...
```

Such definitions need to be provided for all the operators, and for both pairs of `Xvar` and for combinations of `Xvar` and `double`. Overloaded definitions also need to be provided for any intrinsic functions used in the model. Once these class definitions are provided, the original model code can be used to evaluate derivatives automatically where the only requisite changes are the change in type definition, procedures for initialising derivatives (i.e. defining a variable whose derivative is one) and procedures for output of the results.

Specifically, with definitions such as those above, the declaration:

```
Xvar a,b,c;
```

means that, with appropriate initialisation of derivatives, the operation:

```
c = a*b;
```

will calculate both the value of the variable represented by `c`, and its derivatives.

This concept can be extended to automatic calculations of second derivatives, involving objects of the form

$$\frac{\partial^2 x_n}{\partial \alpha_j \partial \beta_k} \quad \text{for } 1 \le j \le J \text{ and } 1 \le k \le K$$

The sets of α_j and β_k may be identical, distinct or overlapping. A common application, with the sets identical α_j and β_k is in assessing ranges of uncertainty associated with calibrations or other optimisations. The following sections involves an analysis of the Brazilian Proposal in terms of derivatives specified for distinct sets. One or more of the α_j is associated with emissions and various β_k correspond to model parameters.

4. THE BRAZILIAN PROPOSAL

In the course of the negotiations that led to the Kyoto Protocol, Brazil tabled a proposal that nations (specifically developed nations) should have emission reduction targets set in proportion to their relative responsibility for the greenhouse effect. Due to a perception of undue complication, this proposal was not included in the draft negotiating text for the Protocol, but was referred to the SBSTA (Subsidiary Body for Scientific and Technical Advice) (under the Framework Convention on Climate Change). Several meetings of experts were convened to work on the issues. This work has continued through an ad hoc working group: MATCH – Modelling and Assessment of Contributions to Climate Change. Further information is available from the MATCH website: www/match-info.net.

In response to scientific criticism of the initial proposal, a refined form was developed (Meira Filho and Miguez, 1998). Summaries of the stages of scientific review and institutional response have been given by Enting and Law (2002: section 5.1). Results from the MATCH working group are reported by den Elzen *et al*., 2005).

An important distinctions was between differences reflecting scientific uncertainties and differences that would arise from specific policy choices for which scientific criteria would not provide a solution. The key policy choices that would need to be made in applying the Brazilian Proposal are the choices of:

indicator — which quantity is attributed and at what time (or over what time interval)?;

attribution group — which emissions (by gases and/or sector) have their climate effects attributed?

attribution period — what periods of emissions are included in the attribution? In particular, should emissions from early periods be excluded because of (a) reduced responsibility due to lesser understanding of the greenhouse effect, and/or (b) poor quality emissions data for input to attribution?

In the present study, we shall follow the original form of using T_τ, the temperature increase at time τ, as the indicator but consider evaluation at various years: $\tau = 2000$, 2050 and 2100. The attribution will consider CO_2 and (in less detail) CH_4. The formalism described below allows us to present results that can be related to a range of attribution periods — the attribution period does not need to be prespecified.

Much of the technical research on the significance of these choices has considered projected emissions over the 21st century. This has had the practical advantage that issues of scientific methodology can be explored without the (justifiable) negative response that would occur if preliminary methodolgies were purporting to attribute responsibility to individual nations for their actual emissions. For example, the preliminary model in the original version of the Brazilian proposal led to a high estimate of the attribution to the UK, as compared to the USA. Although several errors were identified by Enting (1998), suggesting the UK attribution was exaggerated by a factor of about 3, this high attribution to the UK is still occasionally reported as a greenhouse 'fact'.

Enting (1998) noted that non-linearities in the relation between emissions and temperature change would lead to ambiguity in the way that such temperature change was attributed. As well as the two examples given by Enting, a number of other methodologies have been developed by MATCH working group members. Trudinger and Enting (2005) reviewed seven different approaches against a suite of desirable characteristics and favoured two of these: the **time-slice** method (Enting and Law, 2002) based on the splitting illustrated in Figures 1 and 2; and the **marginal** method obtained by taking derivatives.

Actually the term 'marginal attribution' has been applied to more than one method. Trudinger and Enting (2005) describe a method that is more complicated than that described below and which has no obvious advantages compared to the simpler method.

Conceptually, the simpler form of marginal attribution (J. Gundermann, *pers. comm.*) is obtained by taking T_τ as a functional of emissions, expressed as

$$T[E] \quad \text{with} \quad E(t) = \sum_k (1+\alpha_k) E_k(t)$$

and defining the attribution at time τ to group j as

$$T_{\tau:j} = \frac{\partial T}{\partial \alpha_j} \quad \text{for all } \alpha_k = 0$$

One can define a normalised attribution as

$$T_{\tau:j(\mathrm{norm})} = T_\tau \times T_{\tau:j} / \sum_k T_{x:k}$$

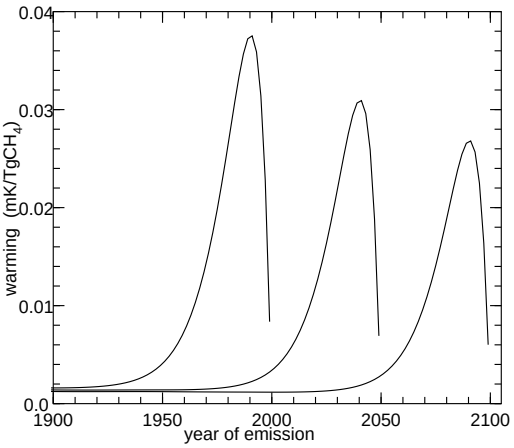

Figure 4. Curves $S_{2000}(t)$, $S_{2050}(t)$ and $S_{2100}(t)$ giving the warming (in milliKelvin per teragram of methane) in the years 2000, 2050 and 2100 due to CH_4 emissions over time.

or relative attribution as

$$T_{\tau:j\%} = 100 T_{\tau:j} / \sum_k T_{\tau:k}$$

However, we can also write the (infinitesimal) perturbation to emissions using the additive form:

$$T[E(t)] \quad \text{with} \quad E(t) = \gamma(t) + \sum_k E_k(t)$$

which leads to the form

$$T_{\tau:j} = \int_{t_0}^{x} E_j(t) S_\tau(t)\, dt \qquad (4)$$

where $S_\tau(t)$ is the functional derivative (a special case of the Frechet derivative) of T_τ with respect to $\gamma(t)$. Knowledge of the single sensitivity function, $S_\tau(t)$, enables us to calculate any or all of the $T_{\tau:j}$ for any attribution period that lies within the domain for which $S_\tau(t)$ is calculated. The use of $S_\tau(t)$ also provides a convenient framework for propagating uncertainties in the emission inventory through to the indicator $T_{\tau:j}$.

For a single indicator time, τ, calculation of $S_\tau(t)$ as a function of t would be most efficiently performed using the adjoint model. The calculations presented here actually used repeated integrations of the tangent linear model. The convenience of having $S_\tau(t)$ (and the ability to capture results for several values of τ) helps compensate for the inefficiency.

Figures 2 and 4 show the temperature sensitivity curves, $S_\tau(t)$ for CO_2 and CH_4 respectively, for indicator times $\tau = 2000, 2050, 2100$. Note, in particular, that the curves drop as t approaches τ. This is a reflection of the committed-warming effect.

At any point in time, much of the warming from the most recent emissions has not yet happened. Figures 3 and 4 also reflect the lower climatic impact of future emissions due to the partial saturation of the CO_2 and CH_4 absorption lines. Apart from the delay associated with unrealised warming, the warming effect of methane is mainly from recent emissions due to methane's relatively short atmospheric lifetime.

5. SENSITIVITY STUDIES

A series of sensitivity studies of the Brazilian proposal are reported by den Elzen and Schaeffer (2000, 2002) and den Elzen *et al.* (2005), using finite differencing.

Section 4 showed how the attribution quantities such as $T_{\tau:j}$ for nation j can be expressed in terms of a sensitivity function $S_\tau(t)$ that is defined as a functional derivative of the indicator function and evaluated by a tangent linear model or (preferably) an adjoint model.

As noted in the previous section, the sensitivity of the indicator $T_{\tau:j}$ to emission uncertainties can be calculated directly from $S_\tau(t)$. If we wish to consider how sensitive the indicator $T_{\tau:j}$ is to uncertainties in the model parameters then we need to consider the sensitivities of $S_\tau(t)$ with respect to such parameters.

For a model parameter β, we have

$$\frac{\partial}{\partial \beta_k} T_{\tau:j} = \int_{t_0}^{\tau} E_j(t) \frac{\partial}{\partial \beta_k} S_\tau(t)\, dt \qquad (5)$$

Figures 5 and 6, both for CO_2 emissions plot the functions $\frac{\partial}{\partial \beta_k} S_\tau(t)$ for β_1 representing the climate sensitivity (Figure 5) and β_2 representing a parameterised carbon cycle uncertainty (Figure 6).

The climate response expresses temperature as a convolution of the radiative forcing with a response function defined as a sum of two exponentials representing fast and slow components of the climate response. Figure 5 shows the proportional sensitivity of the attribution curves, $S_\tau(t)$ to a_1, the amplitude of the fast component. These are expressed as the change in sensitivity for a 1% change in a_1, i.e. $0.01 \frac{\partial}{\partial a_1}$ of $S_\tau(t)$, again with milliKelvin as the temperature units. Not surprisingly, these curves are similar in shape to the $S_\tau(t)$ curves, with the differences only apparent at long time intervals when the slow component contributes significantly.

Following Enting and Trudinger (2002), the present carbon cycle calculations use the formulation proposed by Joos *et al.*, (1996) which has explicit air-sea gas exchange and biotic CO_2-fertilisation and response function representations for other dynamics

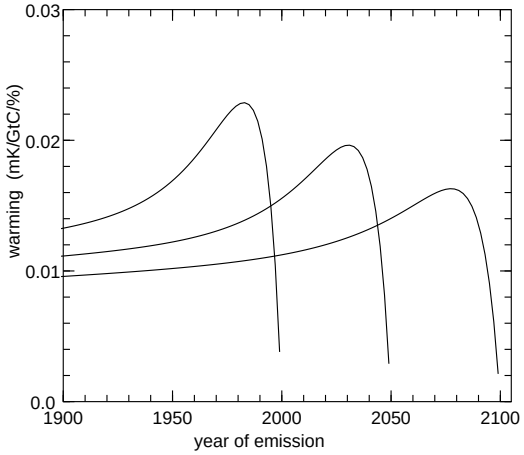

Figure 5. Sensitivity to amplitude of 'fast' climate component of the 2000, 2050, and 2100 temperature responses to CO_2 emissions over time.

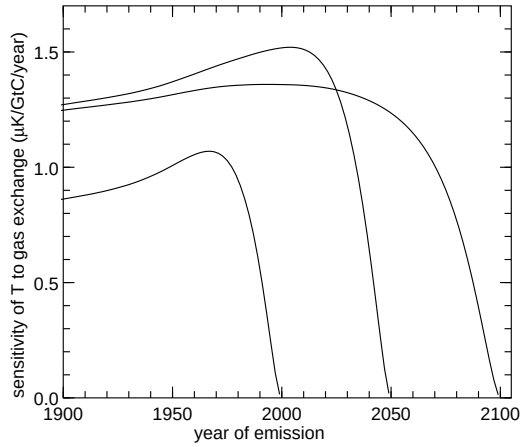

Figure 6. Sensitivity of the curves in Figure 3, $S_{2000}(t)$, $S_{2050}(t)$ and $S_{2100}(t)$ to uncertainties in the air-sea gas turnover time, (in microKelvin per gigatonne of carbon per year exchange time).

of oceans and biota. Rather than look at sensitivities to response function parameters, the example in Figure 6 gives the sensitivity to the air-sea exchange rate, expressed as an atmospheric turnover time, κ. The curves in Figure 6 show $-\frac{\partial}{\partial \kappa}$ of $S_{2000}(t)$, $S_{2050}(t)$ and $S_{2100}(t)$. It will be seen that the pattern of impact of κ varies noticably over time. While these are preliminary results that need more detailed investigation, it seems likely that the differences reflect the shift in relative importance between oceans and biota due to differences in the onset of non-linear saturation effects at larger CO_2 concentrations.

These expressions for sensitivities of $T_{\tau:j}$ represent a reference point. Alternative forms of indicator such as normalised marginal $T_{\tau:j(\mathrm{norm})}$ or relative marginal $T_{\tau:j\%}$ involve ratios that will lead to cancellations.

6. CONCLUSIONS

In the context of the MODSIM conference: this paper represents an example of how a straightforward approach to automatic differentiation can be applied to a real-world problem.

For the Brazilian Proposal: the plots in Figures 3 and 4 provide a new way of representing the marginal attribution of emissions and Figures 5 and 6 represent two of the associated sensitivities. Curves of the type shown in Figures 3 and 4 provide a direct way of relating uncertainties in emission inventories to uncertainties in attribution indicators.

In broader studies of climate change: the methods described here should facilitate other studies of uncertainty in global change. For example, McKibbin and Wilcoxen (2002) claim that their approach is robust with respect to climate model uncertainty. While not implausible, this claim has not yet been quantified and the model analysis approach described here could usefully contribute to such studies.

7. ACKNOWLEDGEMENTS

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