

Carbon Cycle Modelling: Some new techniques

with application to the Brazilian Proposal
& Earth System Model Development

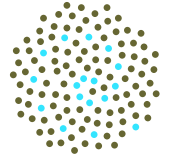
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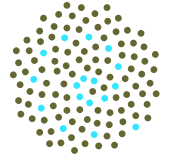


Acknowledgments



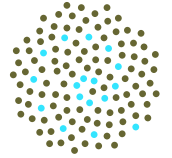
- The Center of Excellence for Mathematics and Statistics of Complex Systems (MASCOS) is funded by the Australian Research Council (ARC).
- My fellowship at MASCOS is supported by CSIRO through a sponsorship agreement.
- The Fortran-90 development is supported by the ARC Earth System Science Network (ARCNESS).
- Collaborators: Cathy Trudinger and YingPing Wang of CSIRO Marine and Atmospheric Research and members of the MATCH working group on the Brazilian Proposal.

Summary



- More than integration:
Model analysis systems
 - Differentiation and some implementations
- Applications of differentiation in:
 - Analysing the Brazilian proposal
 - Calibrating CASACNP terrestrial carbon model (with N and P)

Model Analysis



Most common model calculation is forward projection by (numerical) integration of DEs.

Much model analysis involves differentiation:

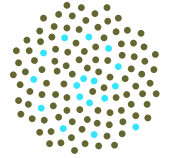
Initialisation Solving for zero rate of change

Sensitivity analysis — derivatives with respect to parameters

Calibration — techniques such as Maximum Likelihood imply optimisations, facilitated by use of derivatives

Data assimilation — real-time model adjustment — dynamic calibration

Data for Carbon Cycle Studies

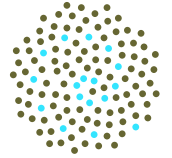


- Air sampling networks interpreted by inverse modelling;
- Satellite data, for quantities such as leaf-area index and phenology
- Terrestrial biosphere models;
- Convective boundary layer measurements;
- Stand-level flux networks;
- Ecosystem experiments;
- Small cuvettes.

From Canadell et al. 2000.

Also satellite data for CO₂ concentrations.

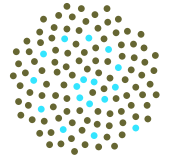
Key characteristics of statistics



- magnitude;
- degree of correlation between components;
- temporal correlation structure;
- spatial correlation structure;
- distribution;
- mismatches in averaging;
- contribution from model representativeness error.

From Raupach et al. 2005

Algorithmic Differentiation (AD)



Differentiation by successive use of chain rule.

For binary operation $c = f(a, b)$,

$$\frac{\partial c}{\partial \alpha} = \frac{\partial f}{\partial a} * \frac{\partial a}{\partial \alpha} + \frac{\partial f}{\partial b} * \frac{\partial b}{\partial \alpha}$$

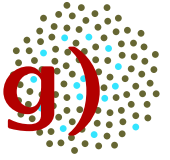
e.g.

$$c = a + b \quad \rightarrow \quad \frac{\partial c}{\partial \alpha} = \frac{\partial a}{\partial \alpha} + \frac{\partial b}{\partial \alpha}$$

$$c = a * b \quad \rightarrow \quad \frac{\partial c}{\partial \alpha} = b * \frac{\partial a}{\partial \alpha} + a * \frac{\partial b}{\partial \alpha}$$

Convert program to code for derivatives, one operation at a time.

Using differentiation (by overloading)

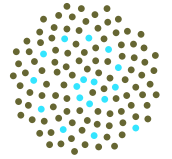


Original

```
double F_co2(double c){  
double a;  
a = log(c/280.0)*5.35;  
return a;  
};  
...  
double cc;  
...  
ff = F_CO2(cc)
```

Transformed

```
Xvar F_co2(Xvar c){  
Xvar a;  
a = log(c/280.0)*5.35;  
return a;  
};  
...  
Xvar cc;  
// Derivatives wrt  
// initial value of cc  
cc.set(280,1);  
...  
ff = F_CO2(cc)
```

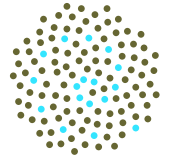
Class Definitions

Fragment of C++ class definition (300 lines) to implement 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;} ;
...
```

Tangent Linear Model (TLM)



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

we can define sensitivities as

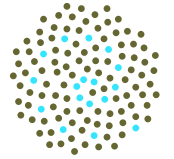
$$y_j = \frac{\partial}{\partial \alpha} x_j \quad \text{for } j = 1, N \quad \text{or} \quad y_{j,p} = \frac{\partial}{\partial \alpha_p} x_j$$

to give 'tangent linear model(s)':

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

$$\frac{d}{dt}y_{m,p} = \frac{\partial}{\partial \alpha_p} g_m(\{x_k\}, \alpha, t) + \sum_n \frac{\partial}{\partial x_n} g_m(\{x_k\}, \alpha, t) y_{n,p}$$

Adjoint (of TLM)



$$\frac{d}{dt}y_{m,p} = \frac{\partial}{\partial \alpha_p} g_m(\{x_k\}, \alpha, t) + \sum_n \frac{\partial}{\partial x_n} g_m(\{x_k\}, \alpha, t) y_{n,p}$$

$$\frac{d}{dt}y_{m,p} = f_{m,p}(t) + \sum_n g_{m,n}(t) y_{n,p}$$

TLM is **linear** and therefore has a (linear)

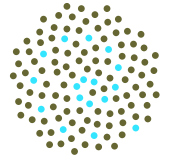
Green's function operator which has an adjoint.

Jacobian is projection of operator onto matrix.

$J_{k,1}$ gives $\frac{\partial v_k}{\partial u_1}$: carry forward single set of $\frac{\partial x_m}{\partial u_1}$

$J_{1,j}$ gives $\frac{\partial v_1}{\partial u_j}$: carry backward single set of $\frac{\partial v_1}{\partial x_m}$

Brazilian Proposal

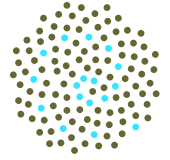


Tabled by Brazil during negotiations leading to Kyoto Protocol — Flicked-passed to Subsidiary Body for Scientific and Technical Advice (SBSTA).

Proposes that emission reduction targets should be proportional to nation's relative responsibility for the greenhouse effect.

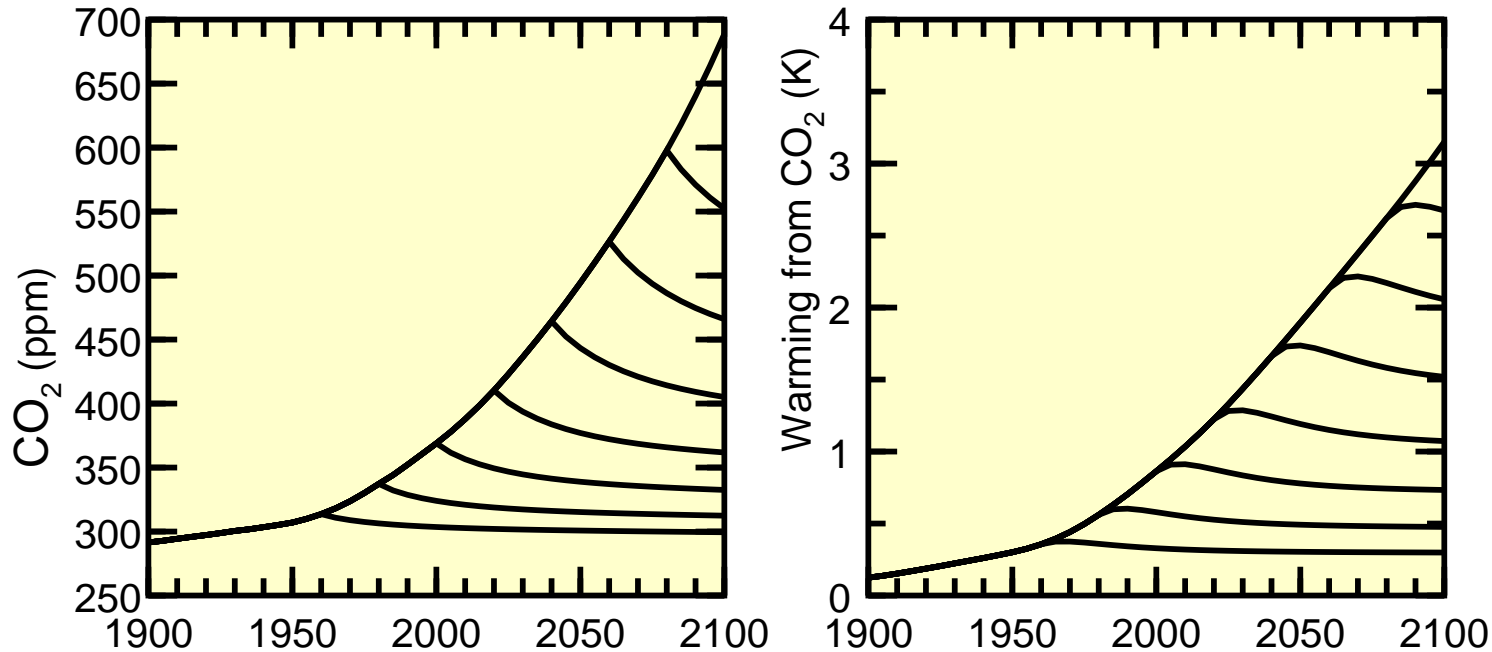
Issues:

- Indicator? What quantity is used as a measure of the greenhouse effect?
- For what period of emissions is responsibility attributed?
- How are non-linear responses attributed?



Timescales

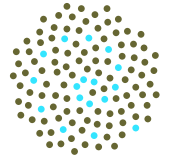
CO₂ concentrations and consequent warming, partitioned according to time of emission.



Lowest bands are from pre-1960 emissions, next from 1960 to 1980 emissions, etc.

Increase in contribution to warming after time of emissions from 'committed warming' effect.

Brazilian Proposal as Derivatives



As example, use indicator $T^* = T_{\text{CO}_2}(2100) =$ warming in 2100 from CO_2 emissions.

T^* is to be attributed to emissions $E_j(t)$ from country j with $E(t) = \sum_j E_j(t)$.

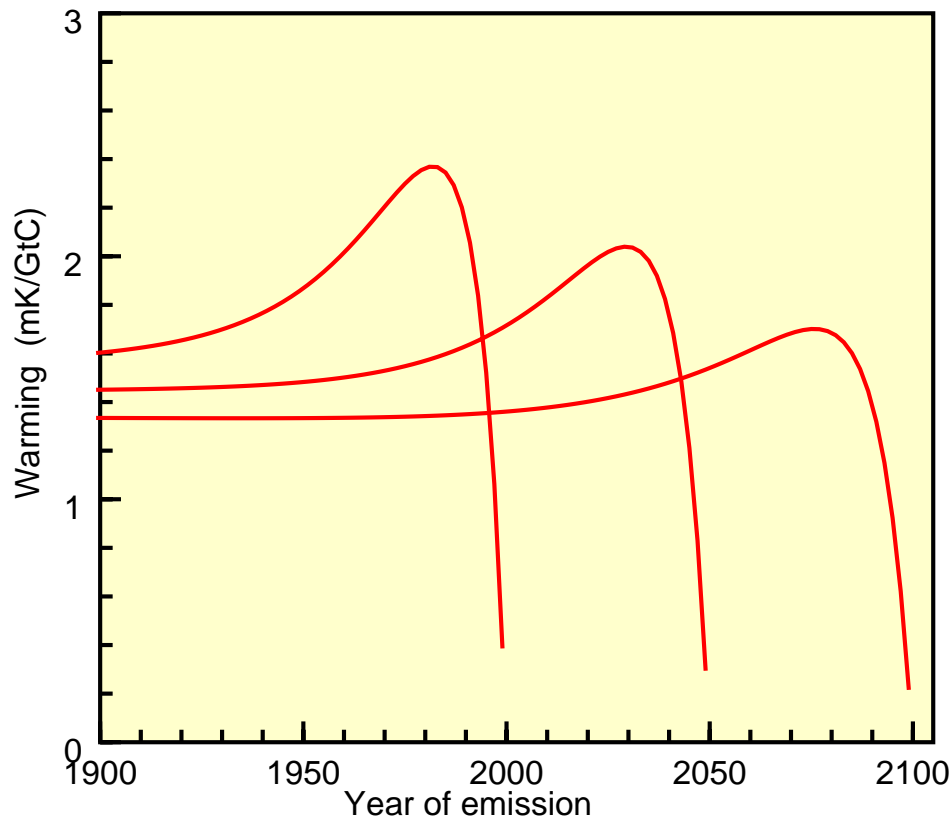
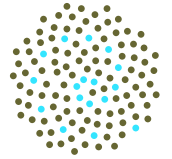
Differential attribution to country j of emissions at time t is

$$\frac{\partial T^*}{\partial E_j(t)} E_j(t) = \frac{\partial T^*}{\partial E(t)} E_j(t) = S(t) E_j(t)$$

where $S(t)$ is a Frechet derivative.

Cumulated attribution: $T_j^* = \int S(t) E_j(t) dt$

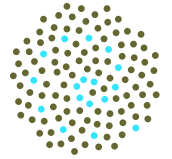
Results: Frechet Derivatives



Assumes IS92a emissions. Represents temperature by response function. Linear responses for ocean and biotic carbon, coupled non-linearly to atmospheric CO₂ (as in CSIRO study).

$$\frac{\partial}{\partial E(t)} T(\tau) \text{ for } \tau = 2000, 2050, 2100.$$

Decrease as $t \rightarrow \tau$ shows 'committed warming'. At any time, warming from the most recent releases is yet to happen.

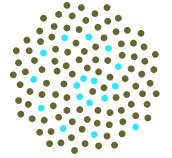


Implications

- For a given indicator, T^* , calculation of $S(t)$ allows attribution to any nation.
- $S(t)$ most efficiently calculated from adjoint model, but for multiple indicator times, tangent linear model not too inefficient.
- Sensitivity of T_j^* to model uncertainties can be obtained as second derivatives.
- Sensitivity of T_j^* to uncertainties in emissions can be obtained as

$$\text{Var}[T_j^*] = \int \int S(t) \text{Cov}[E_j(t), E_j(t')] S(t') dt' dt$$

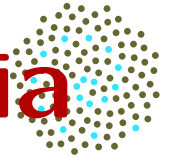
CASACNP AD Project



- Develop Fortran-90/95 implementation of AD by operator overloading;
- Use CASACNP as test case of AD in existing model;
- Explore use of CASACNP derivatives for calibration;
- Document procedure for ARC Network for Earth System Science.

Development funding obtained from ARCNESS for CASACNP and extension to CABLE.

Earth system Modelling in Australia

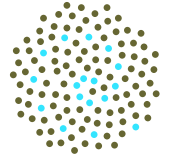


ACCESS: Australian Community Climate and Earth System Simulator.

Bureau of Meteorology, CSIRO and universities.

- UKMO atmosphere (and 4DVAR for NWP)
- Existing ocean used by CSIRO and BMRC (BoM Research Centre)
- Land surface component:
 - existing CSIRO (CABLE)
 - CASA for carbon pools (adding N and P)
 - LPJ for dynamic vegetation

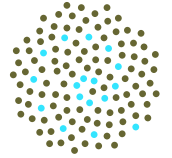
CASACNP



Extend CASA terrestrial carbon model to include nitrogen and phosphorus. (Wang, Field and Houlton).

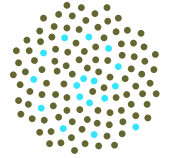
- Initially single region, 8 C pools, 9 N pools, 12 P pools.
- Models response to addition of P, N and competition between N-fixers and non-fixers.
- Validation transect (of soil age) in Hawaii.
- Initial conversion to use AD successful: May 2006 — development on-going.

Putting AD in CASACNP



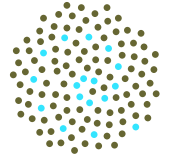
- Added *max* and *min* to initial AD definitions
- Redeclare types of variables
— global edit — not efficient code
- Convert input to write to value – initialise derivatives to zero using compiler option
- Identify variables for differentiation
- Explicit re-writes of .GT. tests using values
- Explicit loops for *array = real* — explicit *1/delt*

Progress on CASACNP



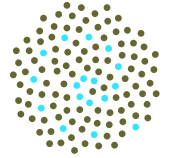
- C++ AD project on Brazilian Proposal: Presented at MODSIM 2005. Proof-of concept for AD by operator overloading.
- Successful proof-of concept of AD by operator overloading in Fortran-95.
- Successful runs using 'brute-force' conversion of CASACNP (May 2006)
- Designing 'vector' version (Spring 2006).
- *Development on-going, supported by ARCNESS*

Parameter Sensitivity: 1



Which parameters most influence the results in the desired application areas?

Parameter Sensitivity: 2



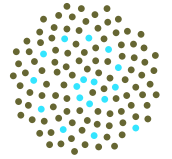
Which parameters influence observable quantities?

(thereby allowing calibration).

Does this set of parameters include all those you need?

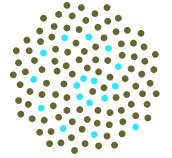
In Bayesian terms, compare s.d. of observations $\times \frac{\partial m}{\partial \alpha}$ with prior s.d. of parameters.

Some general considerations



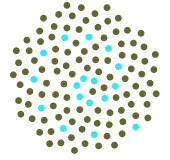
- A carefully designed tool will usually be more effective than a generic tool (Griewank).
(c.f. Unix philosophy: tools that do one thing well, and are combined as required by user)
- The local nature of land-surface processes (carbon and water) suggest that tangent linear model may be as effective as adjoint model.

Future directions



- Incorporate AD into calibration tools.
- Second derivatives in Fortran.
- Explore overloading for Fortran vector operations.
- Develop calibration strategy for CASACNP and other carbon components of Australian Community Climate and Earth System Simulator (ACCESS).

Conclusions



Algorithmic differentiation —

Operator overloading is a straightforward way of developing tangent linear models (and obtaining higher derivatives if needed).

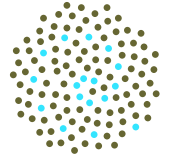
Brazilian Proposal —

Attribution in terms of derivatives is readily calculated using algorithmic differentiation. Higher derivatives give sensitivities.

Global change —

Potential should extend to other analyses of uncertainties in global change.

Further Information



Andreas Griewank, 2000, *Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation*, (SIAM, Philadelphia).

MATCH website (Brazilian Proposal):
<http://www/match-info.net>

I.G. Enting, 2005, *Automatic differentiation in the analysis of strategies for mitigation of global change*, International Congress on Modelling and Simulation, Melbourne, 2005. Ed. A. Zerger and R. M. Argent, 7pp
<http://www.mssanz.org.au/modsim05/papers/enting.pdf>