ARCNESS funding supported work at The University of Melbourne, developing Fortran-90 code for automatic differentiation by operator overloading. While most numerical modelling represents numerical integration of a set of differential equations, differentiation is important in the modelling process for tasks such as, model initialisation, sensitivity analysis, and model calibration.

Algorithmic differentiation is the process of producing computer programs that calculate derivatives that are exact (to machine precision) by applying the rules of calculus to each individual program operation. While this can be done by hand, computerised transformation is more common, in which case the more specific term "automatic differentiation" is often used. Sophisticated tools termed tangent/adjoint compilers exist, with the capability of transforming computer programs into modified programs that can calculate either forward derivatives (tangent models) or backwards derivatives or gradients (termed adjoint models). The latter are particularly useful in generic calibration calculations.

Operator overloading provides an approach to algorithmic differentiation that is much simpler but more restricted than tangent/adjoint compilers. In particular it can only calculate the forward derivatives (tangents) and not the backwards (gradient) derivatives. Algorithmic differentiation is implemented by defining new types of variables that carry both model values and derivative information and defining operators for these variables that calculate values as normal and calculate derivatives by applying the chain rule to propagate derivatives. In principle, such automatic differentiation can be incorporated into an existing program (in any language that supports operator overloading) changing little beyond type specifications and input/output statements.

Prior to this project, work at Melbourne had implemented automatic differentiation in the C++ language, providing a proof of concept of the feasibility and utility of the approach. The ARCNESS funding supported the extension to Fortran-90 for compatibility with ACCESS model development and the extension to allow derivative information to be carried in both real variables and vectors.

The funding from ARCNESS was used to employ Dr. Mark Fielding as a part-time programmer for several months. Dr Fielding's appointment was extended for an extra few weeks using funding (via CSIRO) from the CRC for Greenhouse Gas Technologies, applying the automatic differentiation tools in a study of the marginal utility of carbon sequestration. This was in association with the pilot geosequestration project in the Otway Basin: [http://www.co2crc.com.au/otway/](http://www.co2crc.com.au/otway/)

The capabilities provided by the Fortran code produced for the ARCNESS project are:
* first derivatives for real variables and fixed length vectors;
* second derivatives for real variables;
* suite of test calculations for these capabilities.

These derivative calculations were also linked to generic integration tools and used in modelling work for the Garnaut review, although automatic differentiation played little role in that work. Additional work has involved assessing the computational complexity of tangent vs gradient approaches to identify cases where the tangent capabilities from operator overloading can be usefully deployed. In particular, in global-scale terrestrial carbon modelling, the lack of direct interaction between separate locations makes the tangent approach attractive. Further exploration of this approach has confirmed (a) that the operator overloading approach is compatible with versions of the CASA model being developed for ACCESS, without undue program modification (b) the use of implicit equations allows the use of differentiation for both initialisation and sensitivity analysis without the need to use second derivatives. These studies are continuing.
Publications:


Aspects of the work have also been presented at:
* Workshop on Carbon Cycle Data Assimilation and Mathematical Sciences Research Institute, Berkeley, July 2006;


as well as several research talks in Australia and overseas.