

AUTOMATIC DIFFERENTIATION OF THE COMMUNITY LAND MODEL

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INTRODUCTION

Community Earth System Model (CESM) [1] is a global climate model for simulations of Earth's climate system. Composed of five fully-coupled sub-models of atmosphere, ocean, land, land-ice and sea-ice, it provides state-of-the-art simulations for research of Earth's past, present and future climate states. Community Land Model (CLM) is a sub-model of the CESM for simulations of energy fluxes within the land biogeophysics, chemical compound fluxes within the land biogeochemistry and water fluxes within the land hydrology.

One of the goals of the modeling efforts is to improve the accuracy of climate simulations. Using a model in the diagnostic mode enables modelers to compare and validate the model's results with past climate data. Validation of diagnostic simulations leads to increased confidence in the prognostic simulations of the future climate, which in turn supports regulatory climate policy decisions.

Climate simulations are based on complex numerical analysis and very large data sets. A simplifying abstraction of a climate model is to view it as a composition of functions that model individual climate processes. Each function accepts multiple inputs and produces multiple outputs. The overall composition of functions acts on the initial climate parameters and produces a new state at the end of one simulation step. The new state becomes an input to the model at the next computation step. If the model properly captures key characteristics of the climate dynamics, then there should be no growing discrepancies between the modeled and actual climate states with the progression of time-steps.

Due to the complexity of climate processes, modeling is an approximation effort with each improvement intended to reduce the error in the functional transformation of inputs to outputs. One of the techniques for reduction of errors and improvement in the confidence in model simulations is to compute derivatives of functions. A derivative provides a measure of sensitivity of a function's output to changes in its input. In the context of multiple inputs and outputs, partial derivatives provide an additional measure of which input a function's output is most sensitive to. The sensitivities reduce the uncertainty and allow a modeler to focus on key characteristics of a model.

Automatic differentiation (AD) [2] computes a derivative of a function's program by computing the derivatives of individual operations and propagating derivative values using chained accumulation.

While AD is a major improvement over symbolic or finite differentiation, which can introduce round-off errors, it can reduce the efficiency of the original program with respect to execution time and memory due to the calculation and storage of (intermediate) derivatives. The basic direction of AD research is to improve the efficiency of differentiation. A practical direction is to apply AD to a wide spectrum of real-world numerical computations.

EXPERIMENT

In the case of the community land model, our focus is on the growth of crops and the parameters affecting the crop harvest such as carbon and nitrogen within crop roots, leaves, stems and organs. Proper modeling of crop growth can have significant impact on crop cultivation.

The primary obstacle to the differentiation of the land/crop model is the size of the code base (~70K lines of code) and the complexity of language features (Fortran 90). Further, the code is coupled with parallelization routines of MPI and OpenMP, which serve for efficiency of computation but do not impact the computational core. Therefore, as the initial proof-of-concept, instead of differentiating the entire model, we have focused on applying the AD tool (OpenAD) on a subset of the crop model: allocation of carbon and nitrogen between various crop parts from one time-step to another.

RESULTS

Based on the results of differentiation, we have determined that some parameters are well-quantified and some are not. For example, differentiation with respect to leaf and organ carbon-nitrogen parameters produced greater change in model outputs than doing the same with respect to root and stem carbon-nitrogen parameters. This provided the modelers with better quantification of the effects of inputs on outputs and the overall validity of the model.

REFERENCES

1. UCAR. Community Earth System Model: 2011. <http://www.cesm.ucar.edu>
2. Paul Hovland. Automatic Differentiation of Parallel Programs. PhD Thesis. UIUC, 1997.