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Second-order derivatives of the general-purpose finite element package SEPRAN via source transformation

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Abstract

Second-order derivatives are crucial ingredients to a variety of numerical methods. Often, they are difficult to get with numerical differentiation by divided differencing. Automatic differentiation provides an alternative by a program transformation capable of evaluating Jacobians, Hessians, or higher-order derivatives of functions given in the form of computer programs. SEPRAN is a general-purpose finite element package written in Fortran 77 used in various scientific areas ranging from fluid dynamics to structural mechanics to electromagnetism. By transforming SEPRAN twice using the automatic differentiation tool ADIFOR, second-order derivatives are evaluated without truncation error. Numerical experiments are reported in which second-order derivatives of a flow field with respect to an inflow velocity are computed, demonstrating the feasibility of this approach.

Keywords: Automatic differentiation; Forward mode; ADIFOR; SEPRAN

1. Introduction

In large-scale computational science and engineering, numerical differentiation by divided differencing is often considered to be an attractive option to compute the derivatives of a mathematical function given in the form of a computer program. The reason is its simplicity stemming from the fact that the derivative of a function is solely approximated by repeated evaluations of that function using suitable perturbations of its input. Thus, it is not necessary to implement additional code to evaluate derivatives. However, a disadvantage of divided differencing is the need to experiment with various perturbations. Trading off the cancellation error in finite-precision arithmetic and the inherent truncation error of numerical differentiation is sometimes laborious for first-order derivatives, a phenomenon that may be a serious objection in some applications. For second- and higher-order derivatives, numerical differentiation is notoriously difficult. In contrast, automatic differentiation (AD) not only eliminates the problem of finding a perturbation, but is also capable of evaluating derivatives without truncation error [18,23]; see also the community portal www.autodiff.org.

By using the source-transformation tool ADIFOR [3], we demonstrate that automatic differentiation is feasible to obtain second-order derivative information of a function represented by a non-trivial software package written in Fortran. To this end, we transform the general-purpose finite-element package SEPRAN [24] into a new, "differentiated"

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