Applications of Automatic Differentiation in Computational Fluid Dynamics

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Automatic differentiation (AD) is a powerful computational method that provides a means for computing exact sensitivity derivatives (SD) from existing computer programs for use in multidisciplinary design optimization (MDO) or in sensitivity analysis. The Mathematics and Computer Sciences Division of Argonne National Laboratory and the Center for Research on Parallel Computation at Rice University have developed a pre-compiler AD tool for FORTRAN programs called ADIFOR. The ADIFOR tool has been easily and quickly applied by NASA Langley researchers to assess the feasibility and computational impact of AD in MDO with several different FORTRAN programs. These include a state-of-the-art three-dimensional multigrid Navier-Stokes flow solver for wings or aircraft configurations in transonic turbulent flow. With ADIFOR, the user specifies sets of independent and dependent variables within an existing computer code. ADIFOR then traces the dependency path throughout the code, applies the chain rule to formulate derivative expressions, and generates new code to compute the required SD matrix. The resulting ADIFOR-generated codes have been verified to compute exact nongeometric and geometric SD, for a variety of cases, in less time than is required to compute the SD matrix using centered divided differences.
APPLICATIONS OF AUTOMATIC DIFFERENTIATION IN COMPUTATIONAL FLUID DYNAMICS

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What are Sensitivity Derivatives?

♦ Sensitivity Derivatives (SD) describe how one thing changes with respect to another thing

♦ Example:
  How a car’s speed changes when braking
  – slowly at first, then more quickly
    (how much)
  – speed decreases as braking increases
    (which way)

♦ SD’s describe how much and which way to change the variables in a multidisciplinary design optimization (MDO)
Objectives

- Obtain exact SD using the computational technique of Automatic Differentiation (AD)

- Assess the feasibility and computational impact of AD in a typical MDO problem

The SD Matrix

The SD matrix is given by:

$$SD = \begin{bmatrix}
\frac{\partial o_1}{\partial I_1} & \frac{\partial o_1}{\partial I_2} & \frac{\partial o_1}{\partial I_3} \\
\frac{\partial o_2}{\partial I_1} & \frac{\partial o_2}{\partial I_2} & \frac{\partial o_2}{\partial I_3}
\end{bmatrix}$$

- Sample inputs: Mach number or geometry
- Sample outputs: wing pressure coefficients or grid
- SD matrix required in MDO
Calculation of the SD Matrix

- Divided differences (DD) (baseline + perturbations)
  - Proper step size difficult to determine
  - Truncation & resolution errors
- Hand coding (quasi-analytical) / symbolic manipulators
  - Manual dependency checking
  - Error prone and time consuming
- Automatic Differentiation (AD)
  - Automatic dependency checking and derivative coding
  - Exact derivatives via chain rule
  - Quick & easy; possible speed-up over DD

The AD Tool

- ADIFOR (AD of FORTRAN) / PARASCOPE
  (Argonne National Laboratory and Rice University)

- User identifies dependent and independent variables in program
- ADIFOR follows program flow, traces program dependency paths
- ADIFOR formulates exact derivatives via the chain rule
- ADIFOR generates new code for derivative objects
Potential ADIFOR Use: By Application

Potential ADIFOR Use: By Problem Type
Quasi-Analytic Differentiation

I need sensitivity derivatives ($\frac{df}{dx}$)

Fortran Analysis Code

Quasi-Analytic Differentiation

Fortran Analysis & Sensitivity Analysis Code

I've got them

Automatic Differentiation

I need sensitivity derivatives ($\frac{df}{dx}$)

Specification of Input and Output

Fortran Analysis Code

Standardization

Unoptimized Sensitivity Analysis Code

Improved Sensitivity Analysis Code

I've got them. Would you like ($\frac{df}{dx}$) also?

TODAY

JULY

14

MAY

14

173
Building a Sensitivity Code

Your Computer Code → ADIFOR AD Tool → Code with Sensitivity Derivatives

Objective functions → ADIFOR AD Tool → Code with Sensitivity Derivatives

Design variables → ADIFOR AD Tool → Code with Sensitivity Derivatives

Automatic Differentiation

I need sensitivity derivatives (\frac{df}{dx})

Fortran Analysis Code → ADIFOR → Sensitivity Analysis Code

Specification of Input and Output

I've got them. Would you like \frac{df}{dy} also?

JULY 14
The CFD Codes

- WTCO: wing C-O grid generation
  - Algebraic
  - Transfinite interpolation
- TLNS3D: 3-D thin-layer Navier-Stokes solver
  - Finite-volume, central-differencing
  - Grid sequencing, multigrid
  - Scalar artificial dissipation
  - Baldwin-Lomax turbulence model

ADIFOR Applications in CFD

- WTCO wing grid generation program
  - Independents: thickness, cmax, twist
  - Dependents: grid coordinates (x, y, z)
- TLNS3D Navier-Stokes flow solver
  - Independents: grid coordinates (x, y, z)
  - Dependents: pressure coefficients ($C_p$)
ADIFOR Applications in CFD

- WTCO wing grid generation program
  - Independents: thickness, cmax, twist
  - Dependents: grid coordinates (x, y, z)
- TLNS3D Navier-Stokes flow solver
  - Independents: grid coordinates (x, y, z)
  - Dependents: pressure coefficients (C_p)
- WTCO-TLNS3D coupling via file transfer
  - Grid
  - Grid SD matrix
  - Application of chain rule
    \[
    \frac{\partial(\text{Flow})}{\partial(\text{Sect})} = \frac{\partial(\text{Flow})}{\partial(\text{Grid})} \frac{\partial(\text{Grid})}{\partial(\text{Sect})}
    \]

Computational Results

- ONERA M6 wing planform
- NACA 2412 airfoil sections
- 97 x 25 x 17 grid
- \(M_\infty = 0.84, \alpha = 0.00, \text{Re} = 11.7 \times 10^6\)
- Wing C_p and SD of wing C_p
- Coloring: white/red = large, blue/black = small
- Several geometries:
  - baseline
  - thickness perturbations \(\pm\)
  - cmax perturbations \(\pm\)
  - twist perturbations \(\pm\)
Flow over a wing, M=0.84

- Pressure coefficient (C_p)

SD for wing via AD, M=0.84

- C_p and (d C_p / d twist) for several geometries
SD for wing via AD, M=0.84

- $C_p$ and $(dC_p/dcm_{ax})$ for several geometries

SD for wing via AD, M=0.84

- $C_p$ and $(dC_p/dthick)$ for several geometries
Summary

- Feasibility of using AD in CFD demonstrated

- ADIFOR calculated exact geometric SD for grid-flow coupling similar to MDO problem

- ADIFOR calculated SD through complex algorithm for nonlinear problem

- ADIFOR processing easier & faster than quasi-analytic method

- AD competitive with & more accurate than divided differences

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Sensitivity Derivatives = BETTER

Multidisciplinary Design Optimization = PRODUCTS & PROCESSES

Automatic Differentiation = EASILY, QUICKLY & RELIABLY