ΕΘΝΙΚΟ ΜΕΤΣΟΒΙΟ ΠΟΛΥΤΕΧΝΕΙΟ
Εργαστήριο Θερμικών Στροβιλομηχανών
Μονάδα Παράλληλης Υπολογιστικής Ρευστοδυναμικής & Βελτιστοποίησης

Αυτόματη Διαφόριση (ΑΔ)
Automatic Differentiation (AD)

7ο Εξάμηνο Σχολής Μηχανολόγων Μηχανικών ΕΜΠ
Εισαγωγικό Μάθημα

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AD – Τι χρειάζεται:

$\overrightarrow{b}$ ➡

Κώδικας Ανάλυσης του προβλήματος σε <u>Πηγαία Μορφή</u>. Γραμμένος σε Fortran 77/90 ή ANSI C++.

➡ $F(\overrightarrow{b})$ $(M{=}1)$

$\overrightarrow{F}(\dot{\overrightarrow{b}})$ $(M{>}1)$

$$\Re^N \longrightarrow \Re^M$$

AD – Τρόποι:

Ευθεία ΑΔ
Forward AD

ή

Αντίστροφη ΑΔ
Reverse AD

Υβριδική ΑΔ
Hybrid AD

Διακριτή Συζυγής Μέθοδος
Discrete Adjoint Method

Διαδοχή Τελέσεων (Πράξεων):

Ανεξάρτητες Μεταβλητές

Ενδιάμεσες Εξαρτημένες Μεταβλητές

$$
\left\{
\begin{aligned}
b_{N+1} &= f_{N+1}\left(b_1, \ldots, b_N\right) \\
b_{N+2} &= f_{N+2}\left(b_1, \ldots, b_{N+1}\right) \\
&\vdots \\
b_m &= f_m\left(b_1, \ldots, b_{m-1}\right)
\end{aligned}
\right.
$$

$$F = b_m$$

Ευθεία ΑΔ – Forward AD:

$$b_{N+1} = f_{N+1}(b_1, \ldots, b_N)$$

$$\nabla b_{N+1} = \sum_{i=1}^{N} \frac{\partial f_{N+1}}{\partial b_i} \vec{e}_i$$

$$b_{N+2} = f_{N+2}(b_1, \ldots, b_{N+1})$$

$$\nabla b_{N+2} = \sum_{i=1}^{N} \frac{\partial f_{N+2}}{\partial b_i} \vec{e}_i + \frac{\partial f_{N+2}}{\partial b_{N+1}} \nabla b_{N+1}$$

$$\vdots$$

$$b_m = f_m(b_1, \ldots, b_{m-1})$$

$$\nabla b_m = \sum_{i=1}^{N} \frac{\partial f_m}{\partial b_i} \vec{e}_i + \sum_{i=N+1}^{m-1} \frac{\partial f_m}{\partial b_i} \nabla b_i$$

$$F \equiv b_m$$

$$\nabla F \equiv \nabla b_m$$

Με δαπάνη αρκετής μνήμης!!!

Ευθεία ΑΔ – Forward AD - ΠΑΡΑΔΕΙΓΜΑ:

$$F = b_1 b_2 b_3 b_4$$

$$\Re^4 \rightarrow \Re$$

Ενδιάμεσες Εξαρτημένες Μεταβλητές:

$$\begin{aligned}
b_5 &= f_5(b_1, b_2, b_3, b_4) = b_1 \\
b_6 &= f_6(b_1, b_2, b_3, b_4, b_5) = b_2 b_5 \\
b_7 &= f_7(b_1, b_2, b_3, b_4, b_5, b_6) = b_3 b_6 \\
b_8 &= f_7(b_1, b_2, b_3, b_4, b_5, b_6, b_7) = b_4 b_7 \\
F &= b_8
\end{aligned}$$

$$\begin{aligned}
b_5 &= b_1 \\
\nabla b_5 &= \overrightarrow{e}_1 \\
b_6 &= b_2 b_5 \\
\nabla b_6 &= b_5 \overrightarrow{e}_2 + b_2 \nabla b_5 \\
b_7 &= b_3 b_6 \\
\nabla b_7 &= b_6 \overrightarrow{e}_3 + b_3 \nabla b_6 \\
b_8 &= b_4 b_7 \\
\nabla b_8 &= b_7 \overrightarrow{e}_4 + b_4 \nabla b_7 \\
F &= b_8 \\
\nabla F &= \nabla b_8
\end{aligned}$$

Αντίστροφη ΑΔ – Reverse AD:

Ορίζονται: $$\bar{b}_i = \frac{\partial b_m}{\partial b_i} \qquad (i=N+1,\ldots,m)$$

Εξ ορισμού: $$\bar{b}_m \equiv 1$$

Υπολογίζονται:

$$\bar{b}_i = \sum_{j=i+1}^{m} \frac{\partial b_m}{\partial b_j}\frac{\partial f_j}{\partial b_i} = \sum_{j=i+1}^{m} \bar{b}_j \frac{\partial f_j}{\partial b_i}\ , \qquad \underbrace{i=N+1,\ldots,m-1}_{\text{Εξαρτημένες Μεταβλητές}}$$

$$\bar{b}_i = \sum_{j=N+1}^{m} \frac{\partial b_m}{\partial b_j}\frac{\partial f_j}{\partial b_i} = \sum_{j=N+1}^{m} \bar{b}_j \frac{\partial f_j}{\partial b_i}\ , \qquad \underbrace{i=1,\ldots,N}_{\text{Ανεξάρτητες Μεταβλητές}}$$

Αντίστροφη ΑΔ – Reverse AD:

1. Προς τα Εμπρός (κανονική) Σάρωση:

$$b_i = f_i(b_1, \ldots, b_{i-1}) \ , \quad i = N+1, \ldots, m$$

$$\bar{b}_i = 0 \ , \quad i = 1, \ldots, m-1$$

$$\bar{b}_m = 1$$

2. Προς τα Πίσω (ανάποδη) Σάρωση:

$$do \ j = m, N+1, -1$$

$$do \ i = 1, j-1$$

$$\bar{b}_i = \bar{b}_i + \bar{b}_j \frac{\partial f_j}{\partial b_i}$$

$$enddo$$

$$enddo$$

Αντίστροφη ΑΔ – Reverse AD - ΠΑΡΑΔΕΙΓΜΑ:

$$F = b_1 b_2 b_3$$

$$\Re^3 \longrightarrow \Re$$

Ενδιάμεσες Εξαρτημένες Μεταβλητές:

$$b_4 = f_4(b_1, b_2, b_3) = b_1$$
$$b_5 = f_5(b_1, b_2, b_3, b_4) = b_2 b_4$$
$$b_6 = f_6(b_1, b_2, b_3, b_4, b_5) = b_3 b_5$$

$$\frac{\partial f_3}{\partial b_1} = \frac{\partial f_3}{\partial b_2} = \frac{\partial f_2}{\partial b_1}$$

$$\bar{b}_6 = \frac{\partial f_6}{\partial b_6} \equiv 1$$

$$\bar{b}_5 = \frac{\partial f_6}{\partial b_6}\frac{\partial f_6}{\partial b_5} = \bar{b}_6 \frac{\partial f_6}{\partial b_5}$$

$$\bar{b}_4 = \frac{\partial f_6}{\partial b_6}\frac{\partial f_6}{\partial b_4} + \frac{\partial f_6}{\partial b_5}\frac{\partial f_5}{\partial b_4} = \bar{b}_6 \frac{\partial f_6}{\partial b_4} + \bar{b}_5 \frac{\partial f_5}{\partial b_4}$$

$$\bar{b}_3 = \frac{\partial f_6}{\partial b_6}\frac{\partial f_6}{\partial b_3} + \frac{\partial f_6}{\partial b_5}\frac{\partial f_5}{\partial b_3} + \frac{\partial f_6}{\partial b_4}\frac{\partial f_4}{\partial b_3} = \bar{b}_6 \frac{\partial f_6}{\partial b_3} + \bar{b}_5 \frac{\partial f_5}{\partial b_3} + \bar{b}_4 \frac{\partial f_4}{\partial b_3}$$

$$\bar{b}_2 = \frac{\partial f_6}{\partial b_6}\frac{\partial f_6}{\partial b_2} + \frac{\partial f_6}{\partial b_5}\frac{\partial f_5}{\partial b_2} + \frac{\partial f_6}{\partial b_4}\frac{\partial f_4}{\partial b_2} = \bar{b}_6 \frac{\partial f_6}{\partial b_2} + \bar{b}_5 \frac{\partial f_5}{\partial b_2} + \bar{b}_4 \frac{\partial f_4}{\partial b_2}$$

$$\bar{b}_1 = \frac{\partial f_6}{\partial b_6}\frac{\partial f_6}{\partial b_1} + \frac{\partial f_6}{\partial b_5}\frac{\partial f_5}{\partial b_1} + \frac{\partial f_6}{\partial b_4}\frac{\partial f_4}{\partial b_1} = \bar{b}_6 \frac{\partial f_6}{\partial b_1} + \bar{b}_5 \frac{\partial f_5}{\partial b_1} + \bar{b}_4 \frac{\partial f_4}{\partial b_1}$$

Αντίστροφη ΑΔ – Reverse AD -ΠΑΡΑΔΕΙΓΜΑ:

1

$$\bar{b}_6 \equiv 1 \;,\quad \bar{b}_5 = 0 \;,\quad \bar{b}_4 = 0 \;,\quad \bar{b}_3 = 0 \;,\quad \bar{b}_2 = 0 \;,\quad \bar{b}_1 = 0$$

2

$$\boxed{f_6 = b_3 b_5} \quad \frac{\partial f_6}{\partial b_5} = b_3 \;,\quad \frac{\partial f_6}{\partial b_4} = 0 \;,\quad \frac{\partial f_6}{\partial b_3} = b_5 \;,\quad \frac{\partial f_6}{\partial b_2} = 0 \;,\quad \frac{\partial f_6}{\partial b_1} = 0$$

Σ:

$$\bar{b}_5 = b_3 \;,\quad \bar{b}_4 = 0 \;,\quad \bar{b}_3 = b_5 \;,\quad \bar{b}_2 = 0 \;,\quad \bar{b}_1 = 0$$

3

$$\boxed{f_5 = b_2 b_4} \quad \frac{\partial f_5}{\partial b_4} = b_2 \;,\quad \frac{\partial f_5}{\partial b_3} = 0 \;,\quad \frac{\partial f_5}{\partial b_2} = b_4 \;,\quad \frac{\partial f_5}{\partial b_1} = 0$$

Σ:

$$\bar{b}_4 = b_2 b_3 \;,\quad \bar{b}_3 = b_5 \;,\quad \bar{b}_2 = b_3 b_4 \;,\quad \bar{b}_1 = 0$$

4

$$\boxed{f_4 = b_1} \quad \frac{\partial f_4}{\partial b_3} = 0 \;,\quad \frac{\partial f_4}{\partial b_2} = 0 \;,\quad \frac{\partial f_4}{\partial b_1} = 1$$

Σ:

$$\bar{b}_3 = b_5 \;,\quad \bar{b}_2 = b_3 b_4 \;,\quad \bar{b}_1 = b_2 b_3$$

Αντίστροφη ΑΔ – Reverse AD -ΠΑΡΑΔΕΙΓΜΑ:

Τελική Συνάθροιση Όρων Προς τα Εμπρός:

$$
\begin{aligned}
b_4 &= b_1 \\
\nabla b_4 &= \overrightarrow{e}_1 \\
b_5 &= b_2 b_4 \\
\nabla b_5 &= b_4 \overrightarrow{e}_2 + b_2 \nabla b_4 = b_4 \overrightarrow{e}_2 + b_2 \overrightarrow{e}_1 \\
b_6 &= b_3 b_5 \\
\nabla b_6 &= b_5 \overrightarrow{e}_3 + b_3 \nabla b_5 = b_5 \overrightarrow{e}_3 + b_3 b_4 \overrightarrow{e}_2 + b_3 b_2 \overrightarrow{e}_1
\end{aligned}
$$

Λογισμικό AD:

ADIFOR (Automatic Differentiation of Fortran)
AMC (Tangent linear and Adjoint Model Compiler}
TAF (Transformation of Algorithms in Fortran)
DAFOR (Differential Algebraic Extension of Fortran)
GRESS (Gradient--Enhanced Software System)
Odyssee
TAPENADE
AD01
ADOL-F (Automatic Differentiation of FORTRAN Codes)
IMAS (Integrated Modeling and Analysis System)
OPTIMA90
ADIC (Automatic Differentiation of C Programs)
ADOL-C (Automatic Differentiation of Algorithms written in C/C++)

Εφαρμογή του TAPENADE:

```
C       Generated by TAPENADE     (INRIA, Tropics team)
C  Differentiation of ff in forward (tangent) mode:
C
      SUBROUTINE FF_D(x1, x1d, x2, x2d, x3, x3d, y, yd, z, zd)
      IMPLICIT NONE
      DOUBLE PRECISION x1, x1d, x2, x2d, x3, x3d, y, yd, z, zd
C
      yd = (x1d*x2+x1*x2d)*x3 + x1*x2*x3d
      y = x1*x2*x3
      zd = x1d + x2d + x3d
      z = x1 + x2 + x3
C
      RETURN
      END
```

```
      subroutine ff(x1,x2,x3,y,z)
      implicit double precision(a-h,o-z)
      y = x1*x2*x3
      z = x1+x2+x3
      return
      end
```