TAPENADE

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Outline

1. Presentation of TAPENADE
2. Example Applications
3. Exercise: playing with polygons

The Tapenade AD tool

Tapenade does:

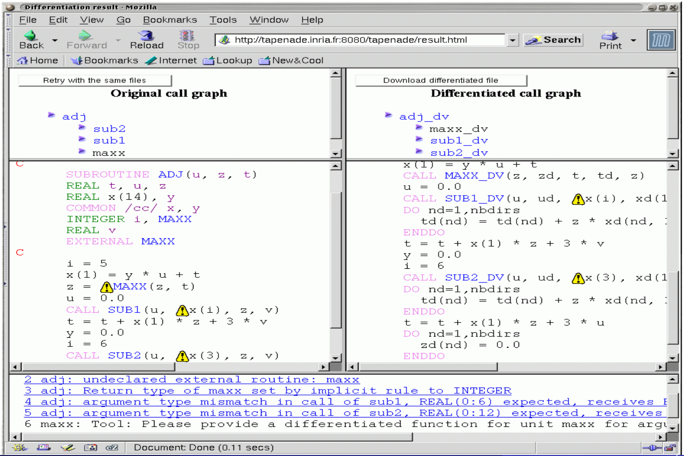
- Automatic Differentiation of imperative programs (F77, F90, C)
- through source transformation
- provides Tangent and Reverse mode
- Reverse strategy: Store-All + Checkpointing on calls
- Extensive source analysis and refinements on the produced source.

Tapenade look and feel

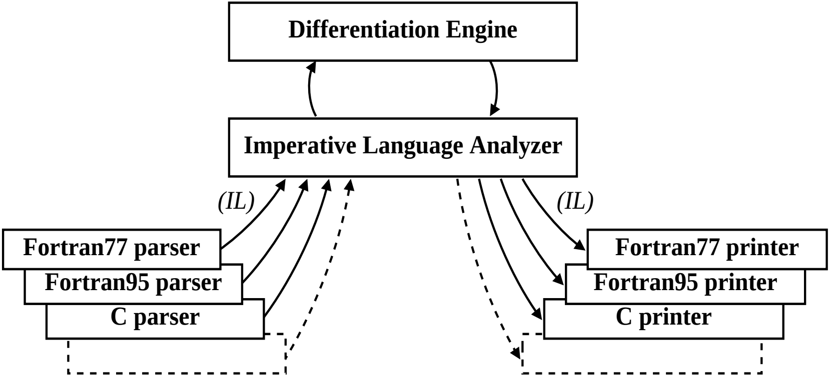
Either:

```
$> tapenade -d -head "FOO(r)/(x y) BAR(q r)/(a)"
file1.f file2.f
```

... or, more colorful:



Tapenade Architecture



- 100 000 lines of Java
- Internal representation: Call Graphs of Flow Graphs
- Differentiates Fortran77-95 and C sources.
- Web server or downloadable executable.

Tapenade Tangent on “Lighthouse”

```
SUBROUTINE EVAL_F   (x,     y     )
DOUBLE PRECISION x(4), y(2), v2



v2 = TAN(x(3)*x(4))


y(1) = x(1)*v2/(x(2)-v2)

y(2) = y(1)*x(2)
END
```

Tapenade Tangent on "Lighthouse"

```
C Differentiation of eval_f in forward (tangent) mode:
C   variations of output variables:  y
C   with respect to input variables:  x
      SUBROUTINE EVAL_F   (x,    y    )
      DOUBLE PRECISION x(4), y(2), v2



      v2 = TAN(x(3)*x(4))


      y(1) = x(1)*v2/(x(2)-v2)

      y(2) = y(1)*x(2)
      END
```

Tapenade Tangent on "Lighthouse"

```
C Differentiation of eval_f in forward (tangent) mode:
C   variations of output variables:  y
C   with respect to input variables:  x
      SUBROUTINE EVAL_F   (x,    y    )
      DOUBLE PRECISION x(4), y(2), v2

      v2d = (xd(3)*x(4)+x(3)*xd(4))
     &       *(1.0+TAN(x(3)*x(4))**2)
      v2 = TAN(x(3)*x(4))
      yd(1) = ((xd(1)*v2+x(1)*v2d)*(x(2)-v2)
     &       -x(1)*v2*(xd(2)-v2d))/(x(2)-v2)**2
      y(1) = x(1)*v2/(x(2)-v2)
      yd(2) = yd(1)*x(2) + y(1)*xd(2)
      y(2) = y(1)*x(2)
      END
```

Tapenade Tangent on “Lighthouse”

```
C Differentiation of eval_f in forward (tangent) mode:
C   variations of output variables:   y
C   with respect to input variables:   x
      SUBROUTINE EVAL_F_D (x,xd,y ,yd)
      DOUBLE PRECISION x(4), y(2), v2
      DOUBLE PRECISION xd(4), yd(2), v2d
      v2d = (xd(3)*x(4)+x(3)*xd(4))
     &        *(1.0+TAN(x(3)*x(4))**2)
      v2 = TAN(x(3)*x(4))
      yd(1) = ((xd(1)*v2+x(1)*v2d)*(x(2)-v2)
     &        -x(1)*v2*(xd(2)-v2d))/(x(2)-v2)**2
      y(1) = x(1)*v2/(x(2)-v2)
      yd(2) = yd(1)*x(2) + y(1)*xd(2)
      y(2) = y(1)*x(2)
      END
```

Tapenade Reverse on “Lighthouse”

```
      SUBROUTINE EVAL_F_B(x, xb, y ,yb)
...   ...   ...
      v2 = TAN(x(3)*x(4))
      y(1) = x(1)*v2/(x(2)-v2)
      y(2) = y(1)*x(2)

      END
```

Tapenade Reverse on "Lighthouse"

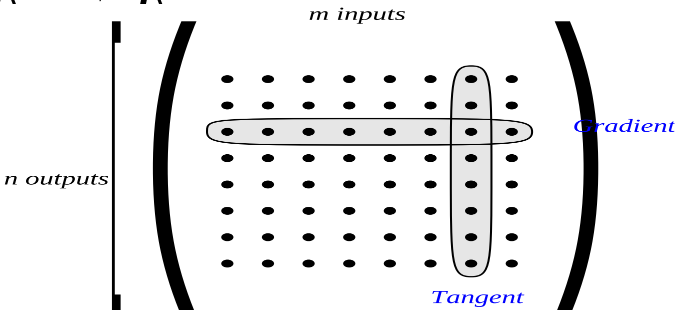
```
C Differentiation of eval_f in reverse (adjoint) mode:
C   gradient, with respect to input variables:  x ...
      SUBROUTINE EVAL_F_B(x, xb, y ,yb)
 ...   ...   ...
      v2 = TAN(x(3)*x(4))
      y(1) = x(1)*v2/(x(2)-v2)
      y(2) = y(1)*x(2)

      END
```

Tapenade Reverse on “Lighthouse”

```
C Differentiation of eval_f in reverse (adjoint) mode:
C   gradient, with respect to input variables:  x ...
       SUBROUTINE EVAL_F_B(x, xb, y ,yb)
  ...   ...   ...
       v2 = TAN(x(3)*x(4))
       y(1) = x(1)*v2/(x(2)-v2)
       y(2) = y(1)*x(2)
       DO ii1=1,4
          xb(ii1) = 0.D0
       ENDDO
       yb(1) = yb(1) + x(2)*yb(2)
       xb(2) = y(1)*yb(2)
       yb(2) = 0.D0
       tempb = yb(1)/(x(2)-v2)
       tempb0 = -(x(1)*v2*tempb/(x(2)-v2))
       xb(1) = xb(1) + v2*tempb
       v2b = x(1)*tempb - tempb0
       xb(2) = xb(2) + tempb0
       yb(1) = 0.D0
       tempb1 = (1.0+TAN(x(3)*x(4))**2)*v2b
       xb(3) = xb(3) + x(4)*tempb1
       xb(4) = xb(4) + x(3)*tempb1
       END
```

Costs of Tangent and Reverse AD

$F \quad : \quad \boldsymbol{R}^m \quad \rightarrow \quad \boldsymbol{R}^n$



- J costs $m * 4 * \mathrm{P}$ using the tangent mode
  Good if $m <= n$
- J costs $n * 4 * \mathrm{P}$ using the reverse mode
  Good if $m >> n$ (e.g $n = 1$ in optimization)

The Store-All strategy in Reverse mode

The Reverse mode uses intermediates in reverse order!

```
y = y + EXP(a)

y = y + a**2

a = 3.5*z
```

The Store-All strategy in Reverse mode

The Reverse mode uses intermediates in reverse order!

```
y = y + EXP(a)

y = y + a**2

a = 3.5*z

zb = zb + 3.5*ab
ab = 0.0

ab = ab + 2*a*yb

ab = ab + EXP(a)*yb
```

The Store-All strategy in Reverse mode

The Reverse mode uses intermediates in reverse order!

```
CALL PUSHREAL8(y)
y = y + EXP(a)
CALL PUSHREAL8(y)
y = y + a**2
CALL PUSHREAL8(a)
a = 3.5*z
CALL POPREAL8(a)
zb = zb + 3.5*ab
ab = 0.0
CALL POPREAL8(y)
ab = ab + 2*a*yb
CALL POPREAL8(y)
ab = ab + EXP(a)*yb
```

⇒ Alternative: Recompute-All (TAF)

⇒ Coarse-grain tradeoff: Checkpointing (on calls)

Refinement: To-Be-Recorded analysis

In reverse AD, not all values must be recorded for the backward sweep.

Variables occurring only in linear expressions do not appear in the differentiated instructions.
$\Rightarrow$ not To-Be-Recorded.

This is a global analysis that must be done on the complete program.

Illustration of TBR analysis

```
CALL PUSHREAL8(y)
y = y + EXP(a)
CALL PUSHREAL8(y)
y = y + a**2
CALL PUSHREAL8(a)
a = 3.5*z
CALL POPREAL8(a)
zb = zb + 3.5*ab
ab = 0.0
CALL POPREAL8(y)
ab = ab + 2*a*yb
CALL POPREAL8(y)
ab = ab + EXP(a)*yb
```

$\longleftarrow$ tbr$= \emptyset$

$\longleftarrow$ tbr$= \{a\}$

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Illustration of TBR analysis

```
CALL PUSHREAL8(y)
y = y + EXP(a)
CALL PUSHREAL8(y)
y = y + a**2
CALL PUSHREAL8(a)
a = 3.5*z
CALL POPREAL8(a)
zb = zb + 3.5*ab
ab = 0.0
CALL POPREAL8(y)
ab = ab + 2*a*yb
CALL POPREAL8(y)
ab = ab + EXP(a)*yb
```

$\longleftarrow$ tbr$= \emptyset$

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$\longleftarrow$ tbr$= \{a\}$

$\longleftarrow$ tbr$= \emptyset$

Tapenade does/doesn't

Tapenade does handle

- all sorts of globals and COMMON's.
- modules, overloading, renaming, interfaces
- structured types ("records")
- pointers and allocation

Tapenade does not handle

- fpp or cpp keys, templates
- deallocation in reverse more
- checkpointing of non-reentrant code
- classes and objects

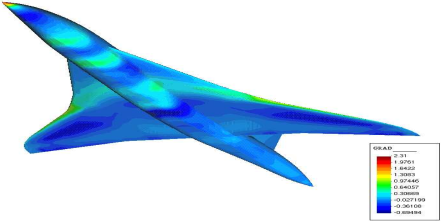
Outline

CFD optimization example

- Cost function: sonic boom below + lift + drag
- Design parameters: plane skin, (2000 `REAL*8`)
- Specific strategy for a steady-state simulation: assembly of the adjoint linear system through AD, then specific solver.
- Performances:
  - Differentiation time: 2 s.
  - Reverse AD slowdown: 7
  - Adjoint slowdown: 4
  - Reverse AD memory use: 58 `REAL*8` per mesh node

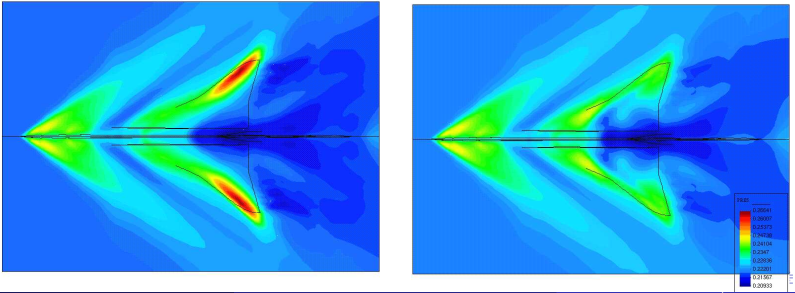
CFD optimization result

AD gradient of the cost function on the skin geometry:



(Dassault Aviation)

Sonic boom under the plane after 8 optimization cycles:

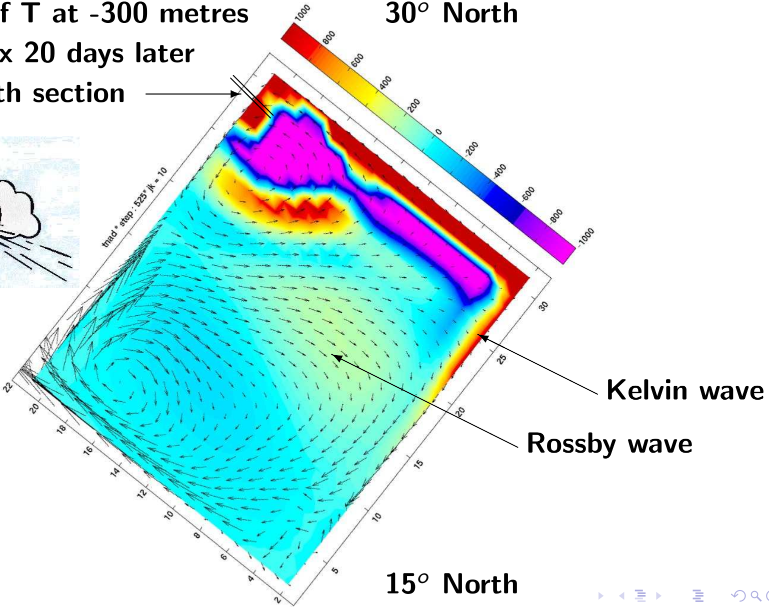


Oceanography example

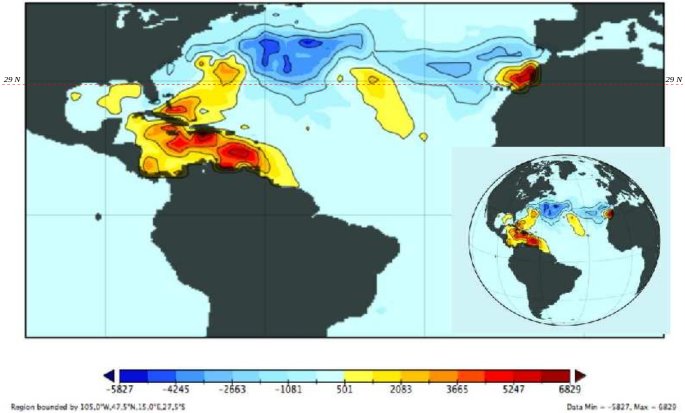
- Code : OPA 9.0. 120000 lines of FORTRAN 95
- Cost function: e.g. some cumulated heat flux
  vs. temperature, salinity. . . at initial state
- Standard reverse AD of complete unsteady simulation
- Differentiation time: 20 s.
- Reverse AD slowdown: 7

OPA 9.0/GYRE

Influence of T at -300 metres on heat flux 20 days later across North section



Gradient OPA-NEMO

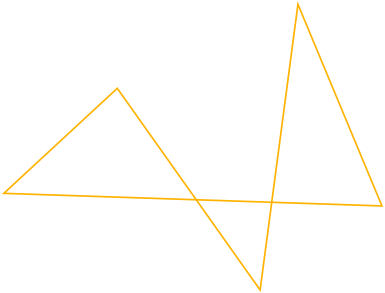


2^o grid cells, one year simulation

Outline

The goal of the game

- Given an initial polygon



- and a program that computes a polygon's surface S and perimeter P,
- move the polygon's vertices to maximize S (P constant),
- using gradient-based optimization.
- Use Tapenade to build the derivative code.

Strategy 1: fixed step size

Use the gradient $(\overline{X}, \overline{Y})$ of the scalar objective function P^2/S with respect to the input parameters (X, Y).

Update the polygon's (X, Y) by

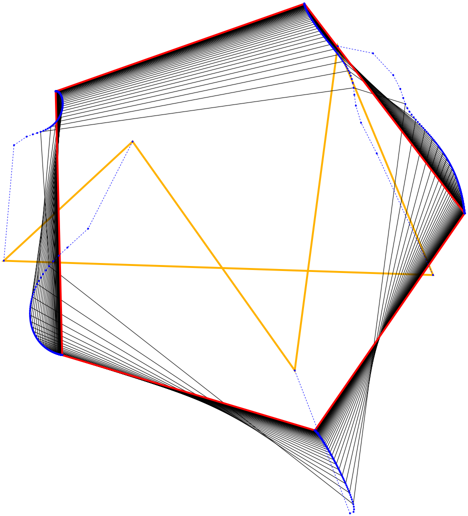
$$\Delta X = \varepsilon \times \overline{X}$$

$$\Delta Y = \varepsilon \times \overline{Y}$$

with a fixed small enough step size ε.

Use Tapenade to produce the code that computes the gradient.
$\Rightarrow$ requires the reverse mode of Tapenade.

Strategy 1: results



714 optimization steps ; time 32

Strategy 2: adaptive step size

Estimate the step size using the Newton method in the gradient direction

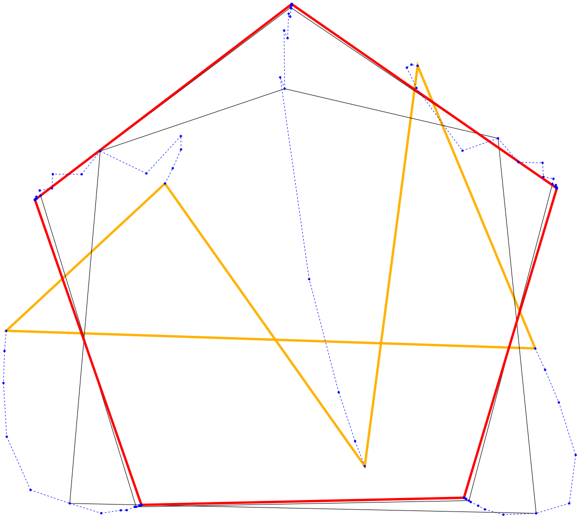
$$\Delta X = p \times \overline{X}$$

$$\Delta Y = p \times \overline{Y}$$

with $p = -\frac{k'}{k''}$, where k is the cost function along the gradient direction.

Use Tapenade to produce the code that computes k' and k''.
$\Rightarrow$ requires the reverse mode of Tapenade and
$\Rightarrow$ requires the 2^{nd}-order tangent on tangent mode of Tapenade.

Strategy 2: results



31 optimization steps ; time 4.6

Strategy 3: true Newton step

The true Newton step $(\Delta X, \Delta Y)$ is in fact the solution of

$$\frac{\partial^2 K}{\partial(\mathtt{X},\mathtt{Y})\partial(\mathtt{X},\mathtt{Y})} \times (\Delta X, \Delta Y) = -\frac{\partial K}{\partial(\mathtt{X},\mathtt{Y})}$$

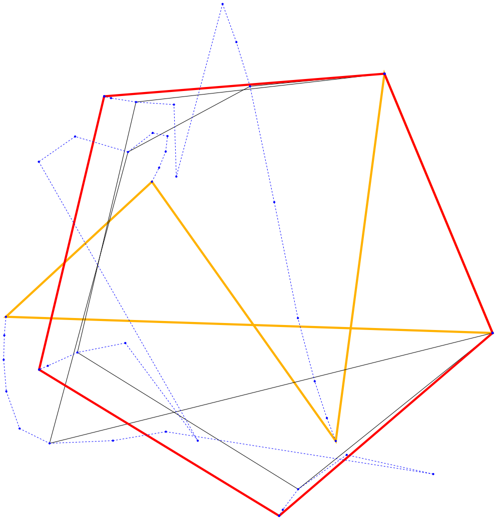
involving the gradient and the Hessian of the cost function K.

Use Tapenade to produce the code that computes

$$\frac{\partial^2 K}{\partial(\mathtt{X},\mathtt{Y})\partial(\mathtt{X},\mathtt{Y})}$$

$\Rightarrow$ requires the reverse mode of Tapenade and
$\Rightarrow$ requires the 2^{nd}-order multi-directional tangent on reverse mode of Tapenade.

Strategy 3: results



15 optimization steps ; time 7.5

... and maybe more if time permits!