# Adjoint approach to optimization using automatic differentiation (AD)

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# Outline

1. Mathematical formulation
2. Computing gradients
3. Quasi 1-D flow
4. Gradient smoothing
5. Quasi 1-D optimization: Pressure matching
6. Example codes

# Outline

# Introduction

- Maturing of high fidelity analysis tools like
  Computational Fluid Dynamics (CFD)
  Finite Element Method (FEM)
- Increase in computational power
- Shift towards optimization and control
- Fluid dynamics
  - Design aircraft wing shape to reduce drag
  - Ship hull shape optimization to reduce drag
  - Minimize unsteady forces through boundary suction/blowing
  - Suppress boundary layer separation
  - Enhance mixing

# Introduction

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  Finite Element Method (FEM)
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# Objectives and controls

- Objective function $J(\alpha) = J(\alpha, u)$
  mathematical representation of system performance
- Control variables $\alpha$
  - Parametric controls $\alpha \in \mathbb{R}^n$
  - Infinite dimensional controls $\alpha : X \to Y$
  - Shape $\alpha \in$ set of admissible shapes
- State variable $u$: solution of an ODE or PDE

$$R(\alpha, u) = 0$$

# Mathematical formulation

- Constrained minimization problem

$$\min_{\alpha} J(\alpha, u) \quad \text{subject to} \quad R(\alpha, u) = 0$$

- Find $\delta\alpha$ such that $\delta J < 0$

$$\begin{aligned} \delta J &= \frac{\partial J}{\partial \alpha}\delta\alpha + \frac{\partial J}{\partial u}\delta u \\ &= \frac{\partial J}{\partial \alpha}\delta\alpha + \frac{\partial J}{\partial u}\frac{\partial u}{\partial \alpha}\delta\alpha \\ &= \left[\frac{\partial J}{\partial \alpha} + \frac{\partial J}{\partial u}\frac{\partial u}{\partial \alpha}\right]\delta\alpha =: G\delta\alpha \end{aligned}$$

- Steepest descent

$$\delta\alpha = -\epsilon G^\top$$

$$\delta J = -\epsilon G G^\top = -\epsilon \|G\|^2 < 0$$

# Mathematical formulation

- Constrained minimization problem

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- Steepest descent

$$\delta\alpha = -\epsilon G^{\top}$$

$$\delta J = -\epsilon G G^{\top} = -\epsilon \|G\|^2 < 0$$

# Sensitivity approach

- Linearized state equation

$$\frac{\partial R}{\partial \alpha}\delta\alpha + \frac{\partial R}{\partial u}\delta u = 0$$

or

$$\boxed{\frac{\partial R}{\partial u}\frac{\partial u}{\partial \alpha} = -\frac{\partial R}{\partial \alpha}}$$

- Solve sensitivity equation iteratively

$$\frac{\partial}{\partial t}\frac{\partial u}{\partial \alpha} + \frac{\partial R}{\partial u}\frac{\partial u}{\partial \alpha} = -\frac{\partial R}{\partial \alpha}$$

- Gradient

$$\frac{\mathrm{d}J}{\mathrm{d}\alpha} = \frac{\partial J}{\partial \alpha} + \frac{\partial J}{\partial u}\frac{\partial u}{\partial \alpha}$$

# Sensitivity approach: Computational cost

- $n$ design variables: $\alpha = (\alpha_1, \ldots, \alpha_n)$
- Solve primal problem $R(\alpha, u) = 0$ to get $u(\alpha)$
- For $i = 1, \ldots, n$
  - Solve sensitivity equation wrt $\alpha_i$

$$\frac{\partial R}{\partial u}\frac{\partial u}{\partial \alpha_i} = -\frac{\partial R}{\partial \alpha_i}$$

  - Compute derivative wrt $\alpha_i$

$$\frac{\mathrm{d}J}{\mathrm{d}\alpha_i} = \frac{\partial J}{\partial \alpha_i} + \frac{\partial J}{\partial u}\frac{\partial u}{\partial \alpha_i}$$

- One primal equation, $n$ sensitivity equations
  Computational cost $= n + 1$

# Adjoint approach

- We have

$$\delta J = \frac{\partial J}{\partial \alpha}\delta\alpha + \frac{\partial J}{\partial u}\delta u \quad \text{and} \quad \frac{\partial R}{\partial \alpha}\delta\alpha + \frac{\partial R}{\partial u}\delta u = 0$$

- Introduce a new unknown $v$

$$\begin{aligned}
\delta J &= \frac{\partial J}{\partial \alpha}\delta\alpha + \frac{\partial J}{\partial u}\delta u + v^\top \left( \frac{\partial R}{\partial \alpha}\delta\alpha + \frac{\partial R}{\partial u}\delta u \right) \\
&= \left( \frac{\partial J}{\partial \alpha} + v^\top \frac{\partial R}{\partial \alpha} \right)\delta\alpha + \left( \frac{\partial J}{\partial u} + v^\top \frac{\partial R}{\partial u} \right)\delta u
\end{aligned}$$

- Adjoint equation

$$\boxed{\left( \frac{\partial R}{\partial u} \right)^\top v = -\left( \frac{\partial J}{\partial u} \right)^\top}$$

- Iterative solution

$$\frac{\partial v}{\partial t} + \left( \frac{\partial R}{\partial u} \right)^\top v = -\left( \frac{\partial J}{\partial u} \right)^\top$$

# Adjoint approach: Computational cost

- $n$ design variables: $\alpha = (\alpha_1, \ldots, \alpha_n)$
- Solve primal problem $R(\alpha, u) = 0$ to get $u(\alpha)$
- Solve adjoint problem

$$\left(\frac{\partial R}{\partial u}\right)^\top v = -\left(\frac{\partial J}{\partial u}\right)^\top$$

- For $i = 1, \ldots, n$
  - Compute derivative wrt $\alpha_i$

$$\frac{\mathrm{d}J}{\mathrm{d}\alpha_i} = \frac{\partial J}{\partial \alpha_i} + v^\top \frac{\partial R}{\partial \alpha_i}$$

- One primal equation, one adjoint equation
  Computational cost = 2, independent of $n$

# Continuous vs Discrete

- Continuous approach:
  - Start with governing PDE $R(\alpha, u) = 0$
  - Derive adjoint PDE and boundary conditions
  - Discretize adjoint PDE and solve
  - Must be re-derived whenever cost function changes
  - Gradient is not consistent: discretization error
- Discrete approach:
  - Start with discrete approximation $R(\alpha, u) = 0$
  - Derive discrete adjoint equations
  - Solve discrete adjoint equations
  - True gradient of discrete solution
  - Can be automated using AD

# Outline

# Techniques for computing gradients

- Hand differentiation
- Finite difference method
- Complex variable method
- Automatic Differentiation (AD)
  - Computer code to compute some function
  - Chain rule of differentiation
  - Generates a code to compute derivatives
  - ADIFOR, ADOLC, ODYSEE, TAMC, TAF, TAPENADE
    see `http://www.autodiff.org`

# Derivatives

- Given a program `P` computing a function $F$

$$\begin{aligned} F \quad : \quad \mathbb{R}^m &\longrightarrow \mathbb{R}^n \\ X &\longrightarrow Y \end{aligned}$$

- build a program that computes derivatives of $F$
- $X$ : independent variables
- $Y$ : dependent variables

# Derivatives

- Jacobian matrix: $J = \left[\frac{\partial y_j}{\partial x_i}\right]$
- Directional or tangent derivative

$$\dot{Y} = J\dot{X}$$

- Adjoint mode

$$\bar{X} = J^\top \bar{Y}$$

- Gradients ($n = 1$ output)

$$J = \left[\frac{\partial y}{\partial x_i}\right]$$

# Forward differentiation

- Program P is a sequence of instructions $F_k$
- $T_o = X$, given
- $k$'th line

$$T_k = F_k(T_{k-1})$$

- Function is a composition

$$F = F_p \circ F_{p-1} \circ \ldots \circ F_1$$

- Chain rule

$$\dot{Y} = F'(X)\dot{X} = F_p'(T_{p-1})F_{p-1}'(T_{p-2}) \ldots F_1'(T_o)\dot{X}$$

$$X, \dot{X} \rightarrow Y, \dot{Y}$$

- $cost(\dot{Y}) = 4 * cost(Y)$

# Differentiation: Example

- A simple example

$$f = (xy + \sin x + 4)(3y^2 + 6)$$

- Computer code, $f = t_{10}$

$$\begin{aligned}
t_1 &= x \\
t_2 &= y \\
t_3 &= t_1 t_2 \\
t_4 &= \sin t_1 \\
t_5 &= t_3 + t_4 \\
t_6 &= t_5 + 4 \\
t_7 &= t_2^2 \\
t_8 &= 3t_7 \\
t_9 &= t_8 + 6 \\
t_{10} &= t_6 t_9
\end{aligned}$$

# F77 code: costfunc.f

```
      subroutine costfunc(x, y, f)
      t1  = x
      t2  = y
      t3  = t1*t2
      t4  = sin(t1)
      t5  = t3 + t4
      t6  = t5 + 4
      t7  = t2**2
      t8  = 3.0*t7
      t9  = t8 + 6.0
      t10 = t6*t9
      f   = t10
      end
```

# Differentiation: Direct mode

- Apply chain rule of differentiation

$$
\begin{aligned}
t_1 &= x \\
t_2 &= y \\
t_3 &= t_1 t_2 \\
t_4 &= \sin(t_1) \\
t_5 &= t_3 + t_4 \\
t_6 &= t_5 + 4 \\
t_7 &= t_2^2 \\
t_8 &= 3 t_7 \\
t_9 &= t_8 + 6 \\
t_{10} &= t_6 t_9
\end{aligned}
\qquad\qquad
\begin{aligned}
\dot{t}_1 &= \dot{x} \\
\dot{t}_2 &= \dot{y} \\
\dot{t}_3 &= \dot{t}_1 t_2 + t_1 \dot{t}_2 \\
\dot{t}_4 &= \cos(t_1) \dot{t}_1 \\
\dot{t}_5 &= \dot{t}_3 + \dot{t}_4 \\
\dot{t}_6 &= \dot{t}_5 \\
\dot{t}_7 &= 2 t_2 \dot{t}_2 \\
\dot{t}_8 &= 3 \dot{t}_7 \\
\dot{t}_9 &= \dot{t}_8 \\
\dot{t}_{10} &= \dot{t}_6 t_9 + t_6 \dot{t}_9
\end{aligned}
$$

- $\boxed{\dot{x} = 1,\ \dot{y} = 0,\ \dot{t}_{10} = \frac{\partial f}{\partial x}}$ and $\boxed{\dot{x} = 0,\ \dot{y} = 1,\ \dot{t}_{10} = \frac{\partial f}{\partial y}}$
- `tapenade -d -vars "x y" -outvars f costfunc.f`

# Automatic Differentiation: Direct mode

```
SUBROUTINE COSTFUNC_D(x, xd, y, yd, f, fd)
t1d = xd
t1 = x
t2d = yd
t2 = y
t3d = t1d*t2 + t1*t2d
t3 = t1*t2
t4d = t1d*COS(t1)
t4 = SIN(t1)
t5d = t3d + t4d
t5 = t3 + t4
t6d = t5d
t6 = t5 + 4
t7d = 2*t2*t2d
t7 = t2**2
t8d = 3.0*t7d
t8 = 3.0*t7
t9d = t8d
t9 = t8 + 6.0
t10d = t6d*t9 + t6*t9d
t10 = t6*t9
fd = t10d
f = t10
END
```

# Backward differentiation

- Program P is a sequence of instructions $F_k$
- $T_o = X$, given
- $k$'th line

$$T_k = F_k(T_{k-1})$$

- Function is a composition

$$F = F_p \circ F_{p-1} \circ \ldots \circ F_1$$

- Chain rule

$$\bar{X} = [F'(X)]^\top \bar{Y} = [F_1'(T_o)]^\top [F_2'(T_1)]^\top \ldots [F_p'(T_{p-1})]^\top \bar{Y}$$

$$X, \bar{Y} \rightarrow \bar{X}$$

- $cost(\bar{X}) = 4 * cost(Y)$

# Differentiation: Reverse mode

- Apply chain rule of differentiation in reverse

$$
\begin{array}{lllllllll}
t_1 & = & x & \quad & \bar{t}_{10} & = & 1 & & \\
t_2 & = & y & & \bar{t}_9 & = & \bar{t}_{10} t_{10,9} & = & t_6 \\
t_3 & = & t_1 t_2 & & \bar{t}_8 & = & \bar{t}_9 t_{9,8} & = & t_6 \\
t_4 & = & \sin(t_1) & & \bar{t}_7 & = & \bar{t}_8 t_{8,7} & = & 3 t_6 \\
t_5 & = & t_3 + t_4 & & \bar{t}_6 & = & \bar{t}_{10} t_{10,6} & = & t_9 \\
t_6 & = & t_5 + 4 & & \bar{t}_5 & = & \bar{t}_6 t_{6,5} & = & t_9 \\
t_7 & = & t_2^2 & & \bar{t}_4 & = & \bar{t}_5 t_{5,4} & = & t_9 \\
t_8 & = & 3 t_7 & & \bar{t}_3 & = & \bar{t}_5 t_{5,3} & = & t_9 \\
t_9 & = & t_8 + 6 & & \bar{t}_2 & = & \bar{t}_7 t_{7,2} + \bar{t}_3 t_{3,2} & = & 6 t_2 t_6 + t_1 t_9 \\
t_{10} & = & t_6 t_9 & & \bar{t}_1 & = & \bar{t}_4 t_{4,1} + \bar{t}_3 t_{3,1} & = & t_9 \cos(t_1) + t_9 t_2
\end{array}
$$

- $\bar{t}_1 = \frac{\partial f}{\partial x}$, $\bar{t}_2 = \frac{\partial f}{\partial y}$
- `tapenade -b -vars "x y" -outvars f costfunc.f`

# Automatic Differentiation: Reverse mode

```
SUBROUTINE COSTFUNC_B(x, xb, y, yb, f, fb)
t1  = x
t2  = y
t3  = t1*t2
t4  = SIN(t1)
t5  = t3 + t4
t6  = t5 + 4
t7  = t2**2
t8  = 3.0*t7
t9  = t8 + 6.0
t10b = fb
t6b = t9*t10b
t9b = t6*t10b
t8b = t9b
t7b = 3.0*t8b
t5b = t6b
t3b = t5b
t2b = t1*t3b + 2*t2*t7b
t4b = t5b
t1b = t2*t3b + COS(t1)*t4b
yb = t2b
xb = t1b
fb = 0.0
END
```

# Direct versus reverse AD

$$F : \mathbb{R}^m \to \mathbb{R}^n$$

- Direct mode
$$cost(J) = m * 4 * cost(P)$$
- Reverse mode
$$cost(J) = n * 4 * cost(P)$$
- Scalar output $F \in \mathbb{R}$, $n = 1$
  - Direct mode gives $\nabla F \cdot \dot{X}$ for given vector $\dot{X}$
  - Reverse mode gives $\nabla F$, hence preferred
- Vector output $F \in \mathbb{R}^n$
  - Direct mode gives $\nabla F \cdot \dot{X}$ for given vector $\dot{X}$
    use for sensitivity equation approach
  - Reverse mode gives $(\nabla F)^\top \cdot \bar{Y}$
    use for adjoint approach

# Issues in reverse AD

- Intermediate variables required in reverse order
- Some variables may be over-written
- Variables may be stored in a stack (PUSH/POP)
- Iterative solvers
  - Only final solution required
  - AD differentiates the iterative loop
  - Intermediate solutions stored in stack
  - Huge memory requirements
  - Not practical for large problems
- Piecemeal differentiation approach (Courty et al., Giles et al.):
  - Modular flow solver
  - Adjoint solver written manually
  - AD for differentiating the modules

# Black-box AD

- cost depends on alpha

```
call ComputeCost(alpha, cost)
```

- Subroutine for cost function

```
subroutine ComputeCost(alpha, cost)
   call SolveState(alpha, u)
   call CostFun(alpha, u, cost)
end
```

- Reverse differentiation using AD

```
tapenade -backward \
         -head ComputeCost \
         -vars alpha \
         -outvars cost \
         ComputeCost.f SolveState.f CostFun.f
```

# Black-box AD

- Diffentiated subroutines:
  ComputeCost_b.f, SolveState_b.f, CostFun_b.f

```
subroutine ComputeCost_b(alpha,alphab,cost,costb)
   call SolveState(alpha, u)
   call CostFun_b(alpha, alphab, u, ub, cost, costb)
   call SolveState_b(alpha, alphab, u, ub)
end
```

- Compute gradient using

```
   costb = 1.0
   call ComputeCost_b(alpha, alphab, cost, costb)
```

- Gradient given by alphab

$$\mathtt{alphab} = \frac{\partial(\mathtt{cost})}{\partial(\mathtt{alpha})}$$

- Solve state equation $R(\alpha, u) = 0$ as steady state of

$$\frac{\mathrm{d}u}{\mathrm{d}t} + R(\alpha, u) = 0, \quad u(0) = u_o$$

- State solver

```
subroutine SolveState(alpha, u)
   u = 0.0
   do while( abs(res) > TOL)
      call Residue(alpha, u, res)
      u = u - dt * res
   end do
end subroutine
```

# AD for iterative problems

Adjoint solver, hand written

```
subroutine SolveState_b(alpha,alphab,u,ub)
resb = 0.0
do while( abs(ub+ub1) .gt. 1.0e-5)
   ub1 = 0.0
   call Residue_bu(alpha,u,ub1,res,resb)
   resb = resb - (ub + ub1)
end do
call Residue_ba(alpha,alphab,u,res,resb)
end subroutine
```

$$\texttt{resb} = \text{Adjoint variable}$$

$$\texttt{ub} = \frac{\partial J}{\partial u}, \quad \texttt{ub1} = \left[\frac{\partial R}{\partial u}\right]^\top v$$

# Adjoint iterative scheme

- Forward iterations linearly stable

$$u^{n+1} = u^n - \Delta t \; R(\alpha, u^n), \quad \Delta t < S(\sigma(R'))$$

- Adjoint iteration

$$v^{n+1} = v^n - \Delta t \left\{ [R'(\alpha, u^\infty)]^\top v^n + \frac{\partial J}{\partial u} \right\}$$

- $[R']^\top$ has same eigenvalues as $R' \implies$ adjoint iterations stable under same condition on $\Delta t$
- Preconditioner for adjoint = (preconditioner for primal problem)$^\top$

# Outline

# 1-D flow equations

- 1-D conservation law

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0, \quad U \in \mathbb{R}^3, \quad F(U) \in \mathbb{R}^3$$

- Finite volume scheme

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} + \frac{F_{i+1/2}^n - F_{i-1/2}^n}{\Delta x} = 0$$

- Update equation

$$U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x} R_i^n, \quad R_i^n = F_{i+1/2}^n - F_{i-1/2}^n$$

# Discrete 1-D adjoint equations

- Finite volume residual for i'th cell, steady state

$$R_i := F_{i+1/2} - F_{i-1/2} = 0$$

- Numerical flux function

$$F = F(X, Y), \quad F_{i+1/2} = F(U_i, U_{i+1})$$

- Perturbation equation

$$\begin{aligned} \delta R_i = \quad & \frac{\partial}{\partial X} F_{i+1/2} \delta U_i + \frac{\partial}{\partial Y} F_{i+1/2} \delta U_{i+1} \\ & - \frac{\partial}{\partial X} F_{i-1/2} \delta U_{i-1} - \frac{\partial}{\partial Y} F_{i-1/2} \delta U_i + \frac{\partial R_i}{\partial \alpha} \delta \alpha \quad = 0 \end{aligned}$$

- Introduce adjoint variable $V_i$ for i'th cell

$$\delta J = \frac{\partial J}{\partial \alpha} \delta \alpha + \sum_i \frac{\partial J}{\partial U_i} \delta U_i + \sum_i V_i^\top \delta R_i$$

# Discrete adjoint equations

- Collecting terms containing $\delta U_i$

$$\delta J = \sum_i \left[ \frac{\partial J}{\partial U_i} \quad + \quad V_{i-1}^\top \frac{\partial}{\partial Y} F_{i-1/2} \right.$$
$$+ \quad V_i^\top \left( \frac{\partial}{\partial X} F_{i+1/2} - \frac{\partial}{\partial Y} F_{i-1/2} \right)$$
$$\left. - \quad V_{i+1}^\top \frac{\partial}{\partial X} F_{i+1/2} \right] \delta U_i \; + \; [\ldots]\delta\alpha$$

- Adjoint equation for i'th cell

$$\left(\frac{\partial J}{\partial U_i}\right)^\top + \left(\frac{\partial}{\partial Y} F_{i-1/2}\right)^\top V_{i-1} \quad + \quad \left(\frac{\partial}{\partial X} F_{i+1/2} - \frac{\partial}{\partial Y} F_{i-1/2}\right)^\top V_i$$
$$- \quad \left(\frac{\partial}{\partial X} F_{i+1/2}\right)^\top V_{i+1} = 0$$

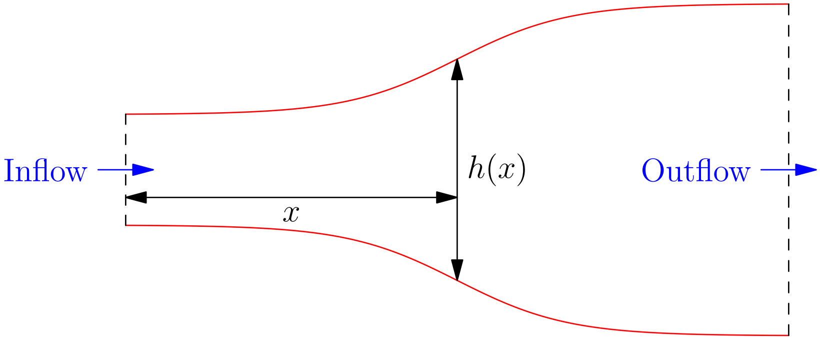
# Example flow solver

```
While u is not converged
  res = 0.0
  fluxinflow(u(1), res(1))
  do i=1,N-1
    fluxinterior(u(i), u(i+1), res(i), res(i+1))
  enddo
  fluxoutflow(u(N), res(N))
  do i=1,N
    u(i) = u(i) - (dt/dx)*res(i)
  enddo
endwhile

cost=0.0
do i=1,N
  costfunc(u(i), cost)
enddo
```

# Example adjoint solver

```
costb=1.0
do i=1,N
  costfunc_b(u(i), ub1(i), cost, costb)
enddo

v=0.0
While v is not converged
  ub2 = 0.0
  fluxinflow_b(u(1), ub2(1), res(1), v(1))
  do i=1,N-1
    fluxinterior_b(u(i), ub2(i), u(i+1), ub2(i+1),
                   res(i), v(i), res(i+1), v(i+1))
  enddo
  fluxoutflow_b(u(N), ub2(N), res(N), v(N))
  do i=1,N
    v(i) = v(i) - (dt/dx)*(ub1(i) + ub2(i))
  enddo
endwhile
```

# Quasi 1-D flow



# Quasi 1-D flow

- Quasi 1-D flow in a duct

$$\frac{\partial}{\partial t}(hU) + \frac{\partial}{\partial x}(hf) = \frac{\mathrm{d}h}{\mathrm{d}x}P, \quad x \in (a,b) \quad t > 0$$

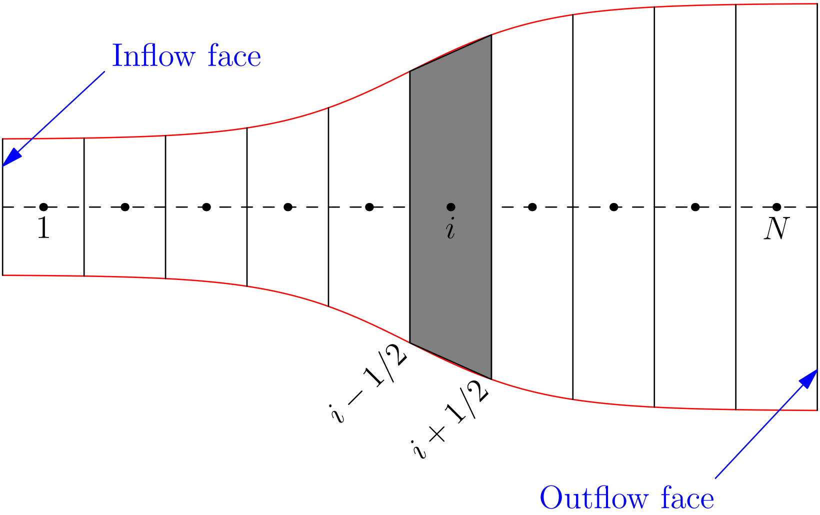
$$U = \begin{bmatrix} \rho \\ \rho u \\ E \end{bmatrix}, \quad f = \begin{bmatrix} \rho u \\ p + \rho u^2 \\ (E+p)u \end{bmatrix}, \quad P = \begin{bmatrix} 0 \\ p \\ 0 \end{bmatrix}$$

$$h(x) = \text{cross-section height of duct}$$

- Inverse design: find shape $h$ to get pressure distribution $p^*$
- Optimization problem: find the shape $h$ which minimizes

$$J = \int_a^b (p - p^*)^2 \mathrm{d}x$$

# Quasi 1-D flow



# Quasi 1-D flow

- Finite volume scheme

$$h_i \frac{\mathrm{d}U_i}{\mathrm{d}t} + \frac{h_{i+1/2}F_{i+1/2} - h_{i-1/2}F_{i-1/2}}{\Delta x} = \frac{(h_{i+1/2} - h_{i-1/2})}{\Delta x} P_i$$

- Discrete cost function

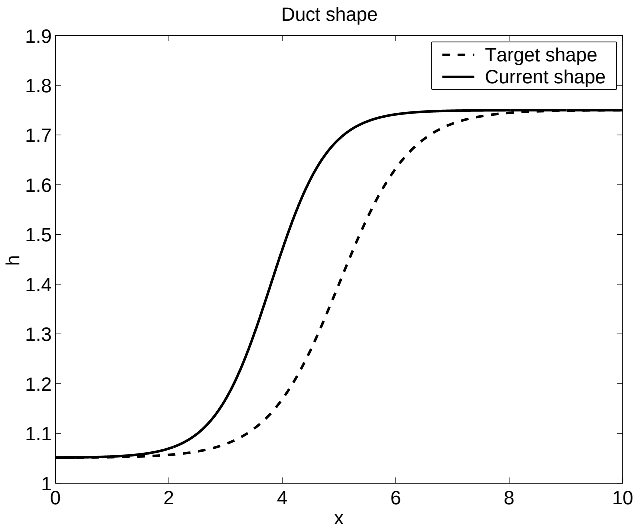
$$J = \sum_{i=1}^{N} (p_i - p_i^*)^2$$

- Control variables

$$h_{1/2}, h_{1+1/2}, \ldots, h_{i+1/2}, \ldots, h_{N+1/2}$$

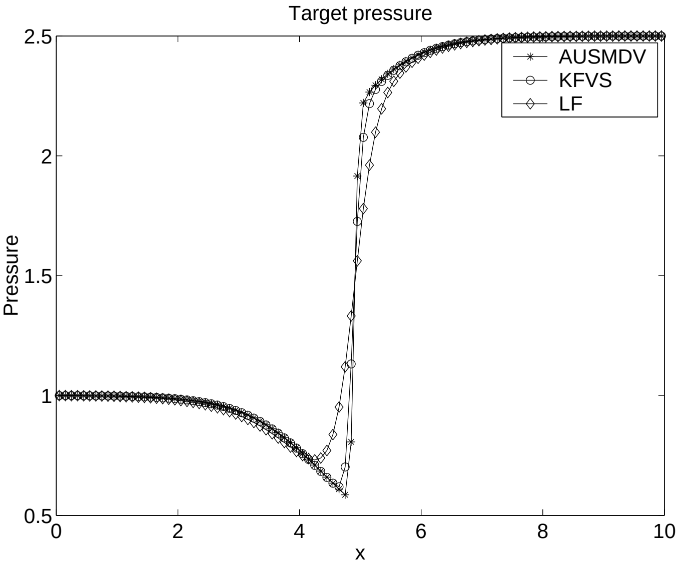
- $N = 100$

# Duct shape

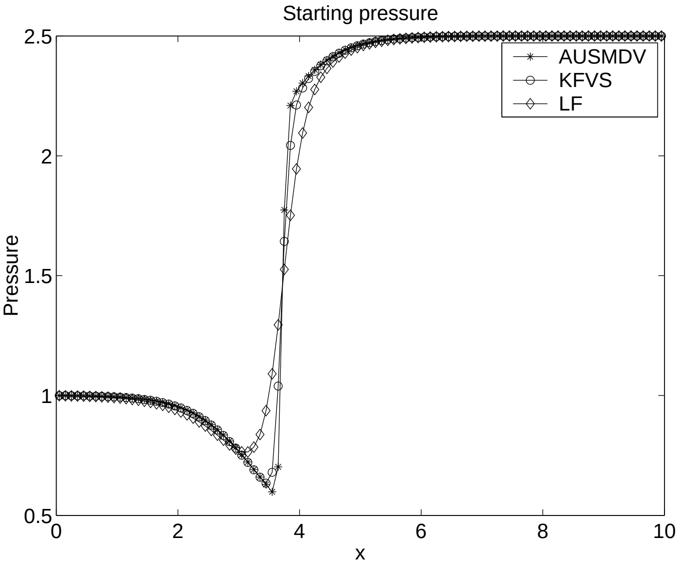


Duct shape
Target shape
Current shape
h
x
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1
0
2
4
6
8
10

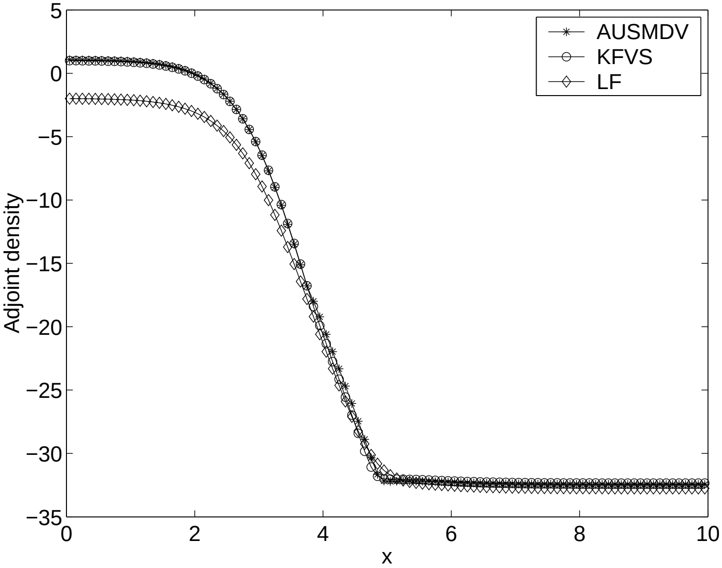
# Target pressure distribution $p^*$



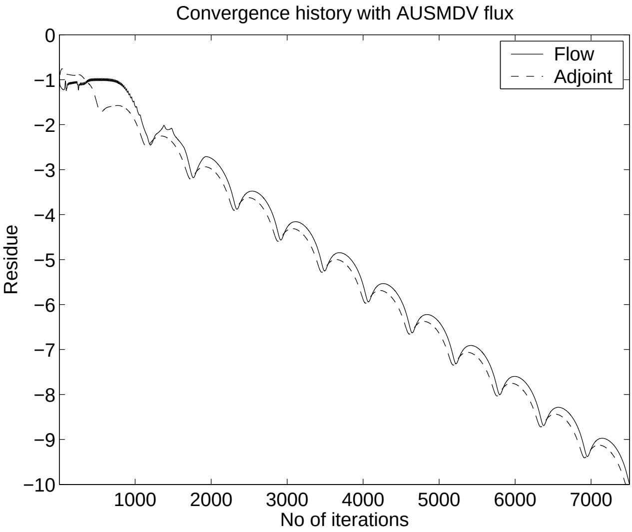
# Current pressure distribution



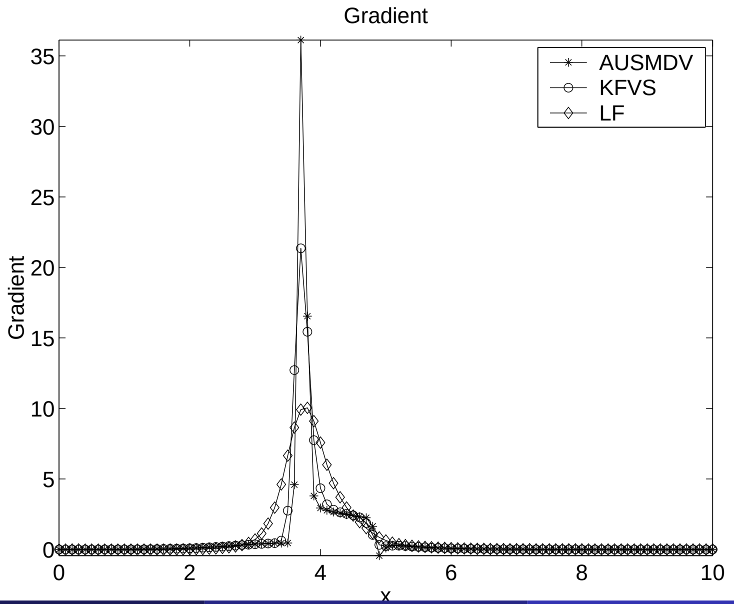
# Adjoint density



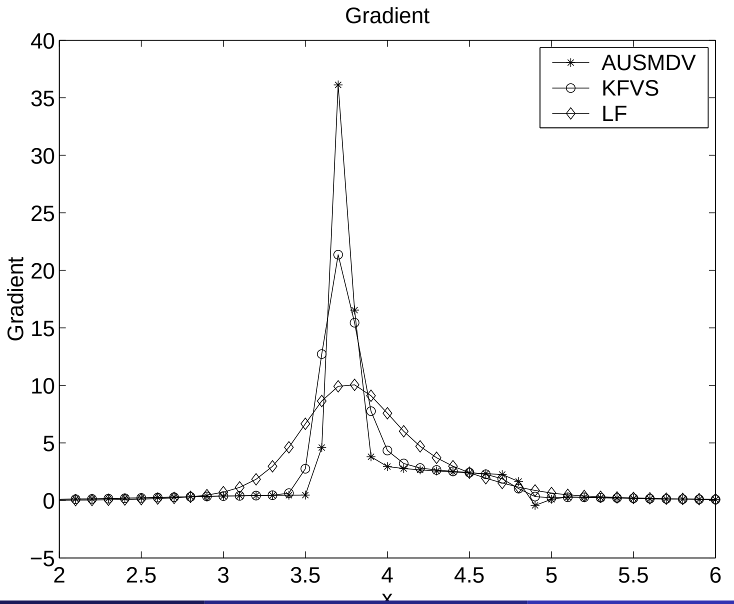
# Convergence history: Explicit Euler



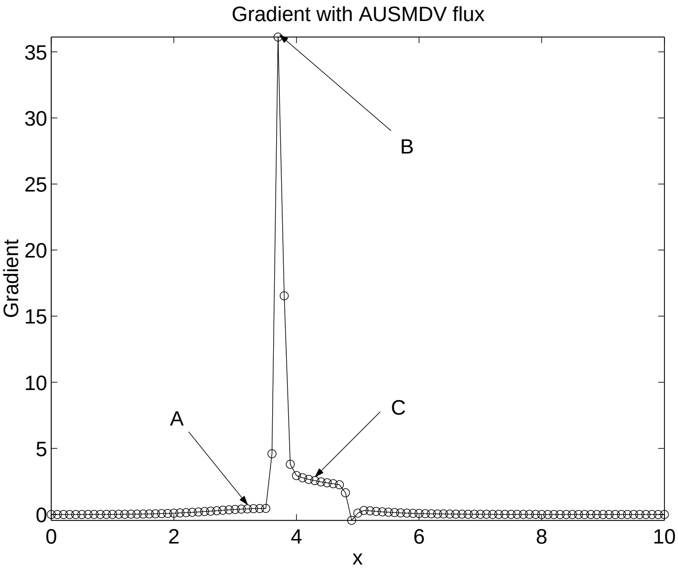
# Shape gradient



# Shape gradient



# Validation of Shape gradient



# Validation of shape gradient

$$\frac{\partial J}{\partial h} \approx \frac{J(h + \Delta h) - J(h - \Delta h)}{2\Delta h}$$

| $\Delta h$ | A | B | C |
|---|---|---|---|
| 0.01 | 0.4191069499 | 35.18452823 | 2.545316345 |
| 0.001 | 0.4231223499 | 36.10982621 | 2.556461900 |
| 0.0001 | 0.4231624999 | 36.11933154 | 2.556573499 |
| 0.00001 | 0.4231599998 | 36.11942125 | 2.556575000 |
| 0.000001 | 0.4231999994 | 36.11942305 | 2.556550001 |
| 0.0000001 | 0.4229999817 | 36.11942329 | 2.556499971 |
| AD | 0.4231628330 | 36.11941951 | 2.556574450 |

# Outline

# Gradient smoothing

- Non-smooth gradients $G$ especially in the presence of shocks
- Smooth using an elliptic equation

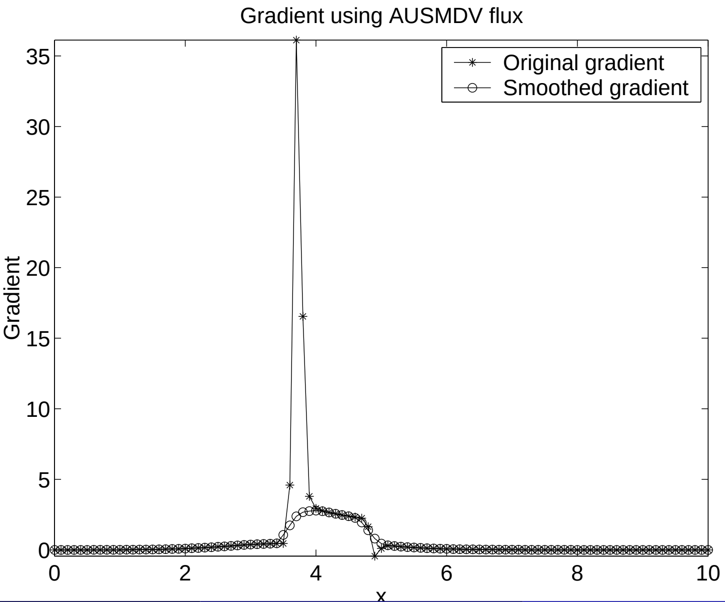
$$\left(1 - \epsilon \frac{\mathrm{d}^2}{\mathrm{d}x^2}\right) \bar{G} = G$$

$$\epsilon_i = \{|G_{i+1} - G_i| + |G_i - G_{i-1}|\} L_i$$

$$L_i = \frac{|G_{i+1} - 2G_i + G_{i-1}|}{\max(|G_{i+1} - G_i| + |G_i - G_{i-1}|, \mathrm{TOL})}$$

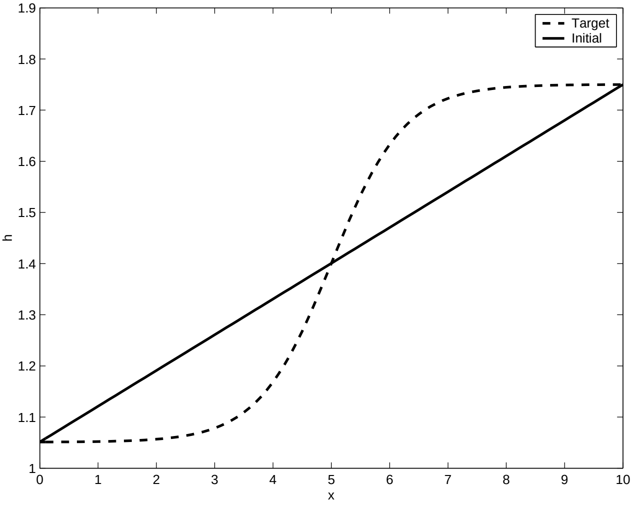
- Finite difference with Jacobi iterations

# Gradient smoothing

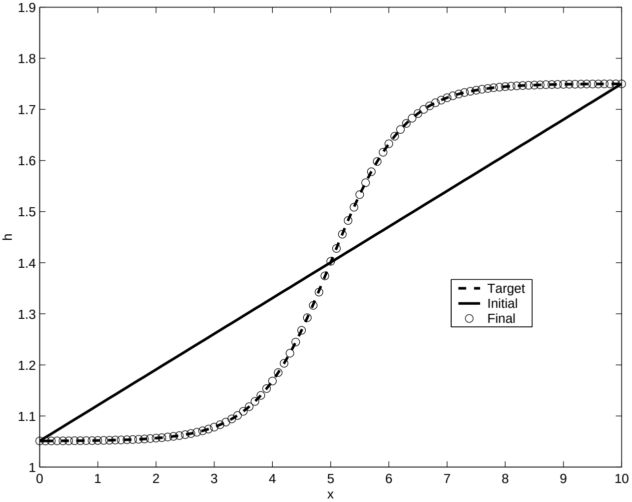


# Outline

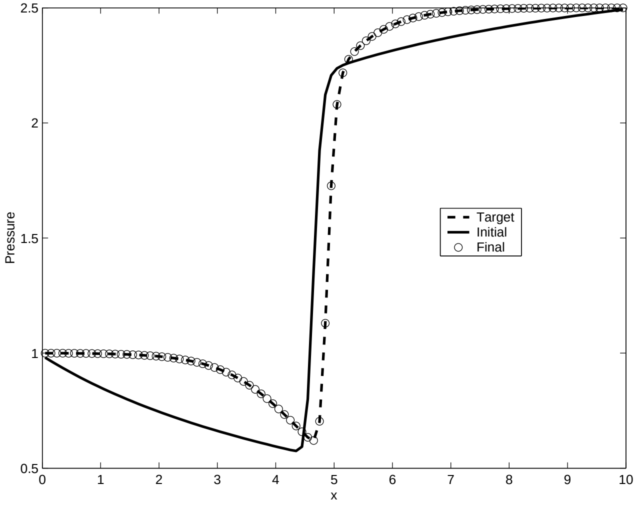
# Quasi 1-D optimization: Shape



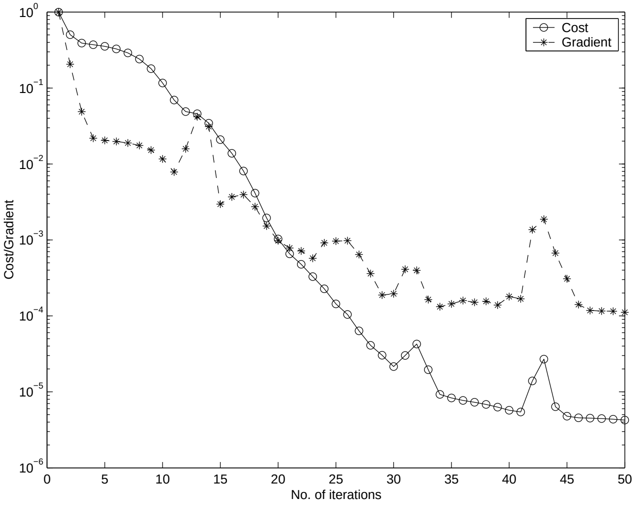
# Quasi 1-D optimization: Final shape



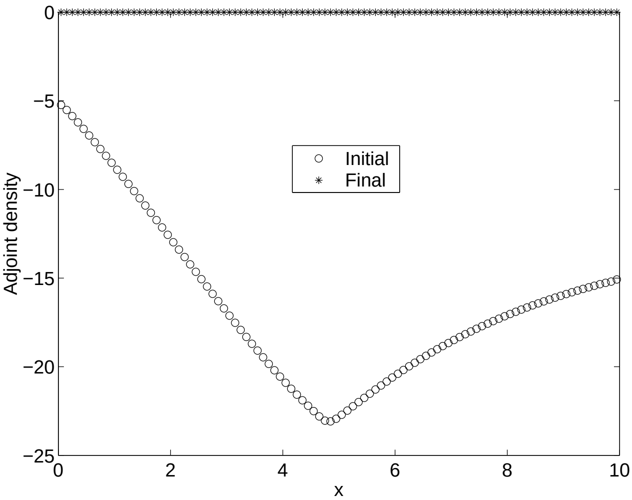
# Quasi 1-D optimization: Pressure



# Quasi 1-D optimization: Convergence



# Quasi 1-D optimization: Adjoint density



# Outline

# AD Tool: Tapenade

- Source transformation tool
- Forward and backward mode
- F77, F90, F95, C (beta as of Nov 2008)
- Free
- `http://www-sop.inria.fr/tropics`

# Example codes

- 1-D example: nozzle flow (TAPENADE)
  http://cfdlab.googlecode.com
- 1-D example: nozzle flow (ADOLC)
  http://cfdlab.googlecode.com
- 2-D example: unstructured grid Euler solver (TAPENADE)
  http://euler2d.sourceforge.net
- 2/3-D example: structured grid Euler solver (TAPENADE)
  http://nuwtun.berlios.de