Adjoint Computation

for Aerodynamic Shape Optimization in MDO context

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University of Trier

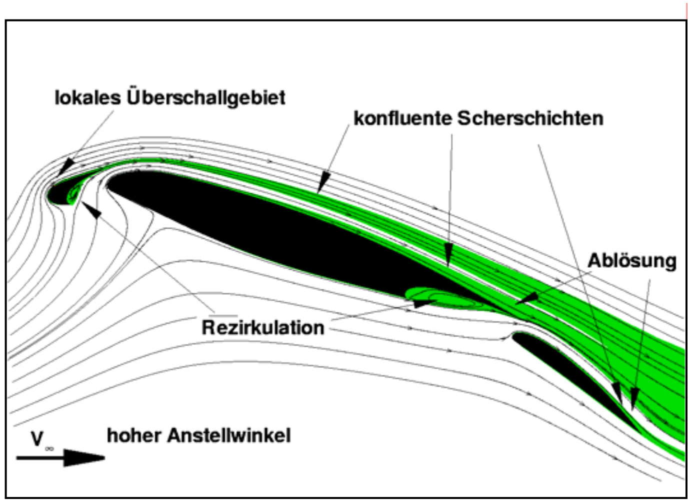
Content of Lecture

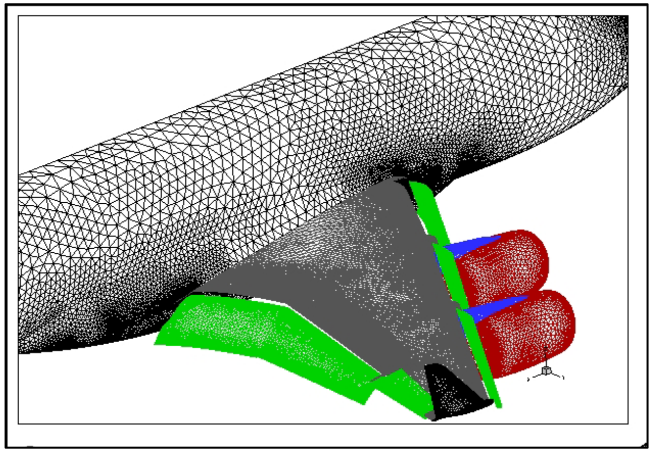
- Why adjoint approaches?
- What is an adjoint approach?
- Continuous and discrete adjoint approaches / solvers
- Validation and Application in 2D and 3D
- Algorithmic / Automated Differentiation (AD)
- Coupled aero-structure adjoint approach
- Validation and application in MDO context
- One shot approaches

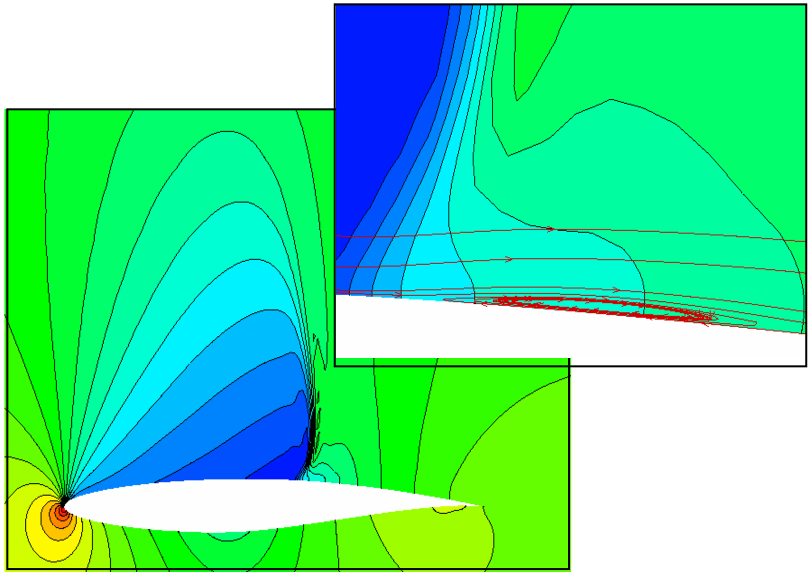
Use of CFD in Aerodynamic Aircraft Design

Requirements on CFD

- high level of physical modeling
  - compressible flow
  - transonic flow
  - laminar - turbulent flow
  - high Reynolds numbers (60 million)
  - large flow regions with flow separation
  - steady / unsteady flows
- complex geometries
- short turn around time





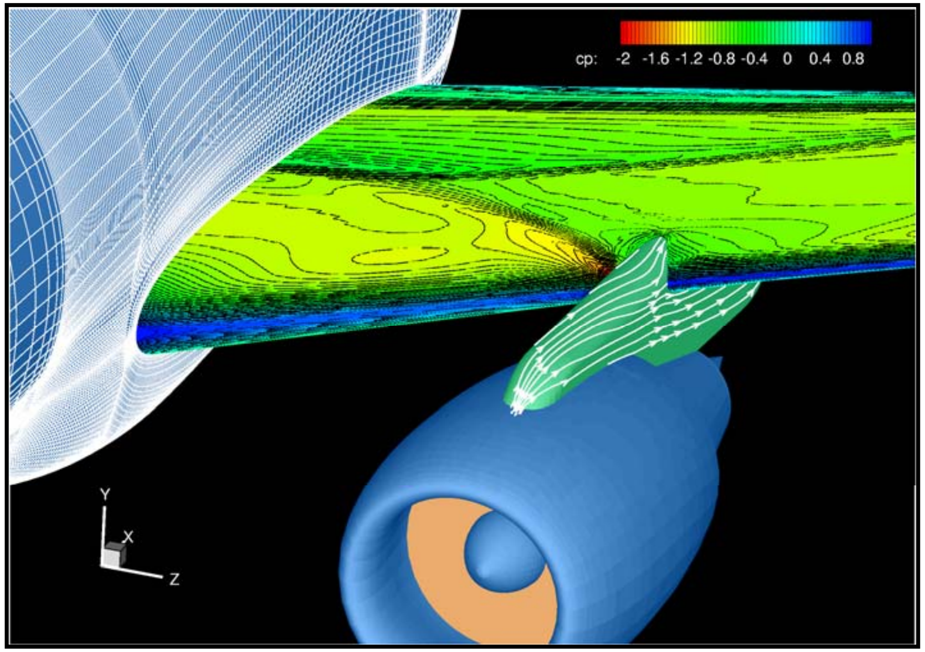


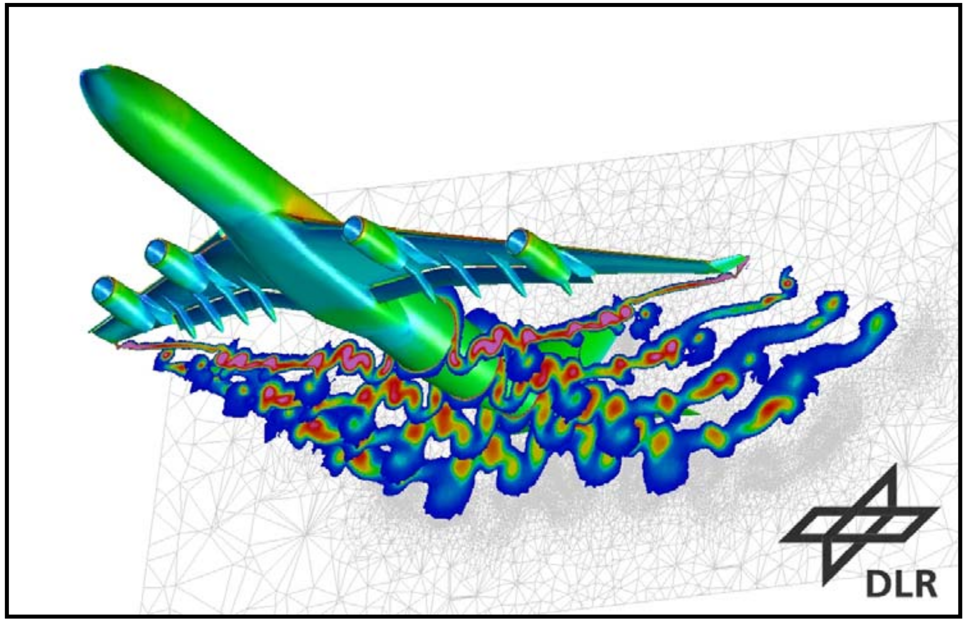
Use of CFD in Aerodynamic Aircraft Design

Consequences

- solution of 3D compressible Reynolds averaged Navier-Stokes equations
- turbulence models based on transport equations (2 – 6 eqn)
- models for predicting laminar-turbulent transition
- flexible grid generation techniques with high level of automation (block structured grids, overset grids, unstructured/hybrid grids)
- link to CAD-systems
- efficient algorithms (multigrid, grid adaptation, parallel algorithms...)
- large scale computations (~ 10 - 60 million grid points)
- …

MEGAFLOW Software





Structured RANS solver FLOWer

- block-structured grids
- moderate complex configurations
- fast algorithms (unsteady flows)
- design option
- adjoint option

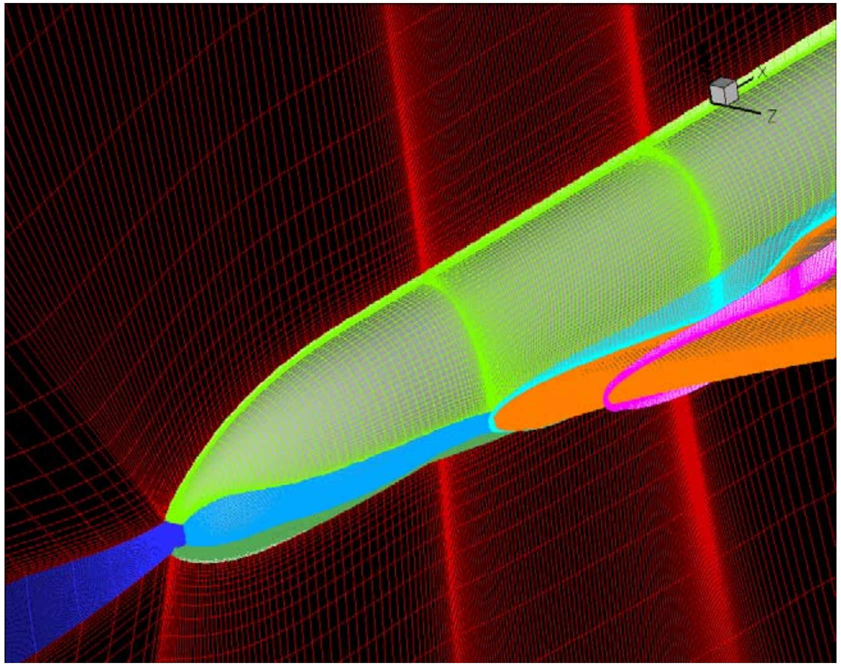
Unstructured RANS solver TAU

- hybrid grids
- very complex configurations
- grid adaptation
- fully parallel software
- adjoint option

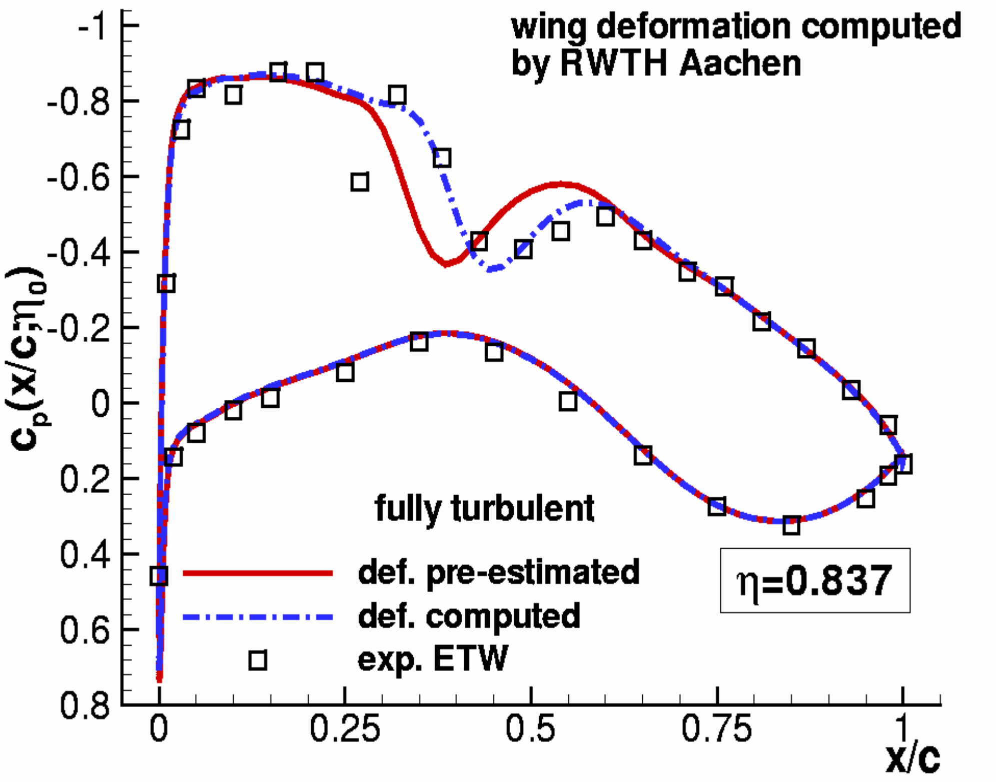
Validation

HiReTT Wing/Body Configuration

- M_∞=0.85, Re=32.5x10^6
- coupled CFD/structural analysis for wing deformation at $\alpha \approx 1.5°$
- FLOWer, kω turbulence model, fully turbulent



3.5 million grid points



Validation
HiReTT Wing/Body Configuration

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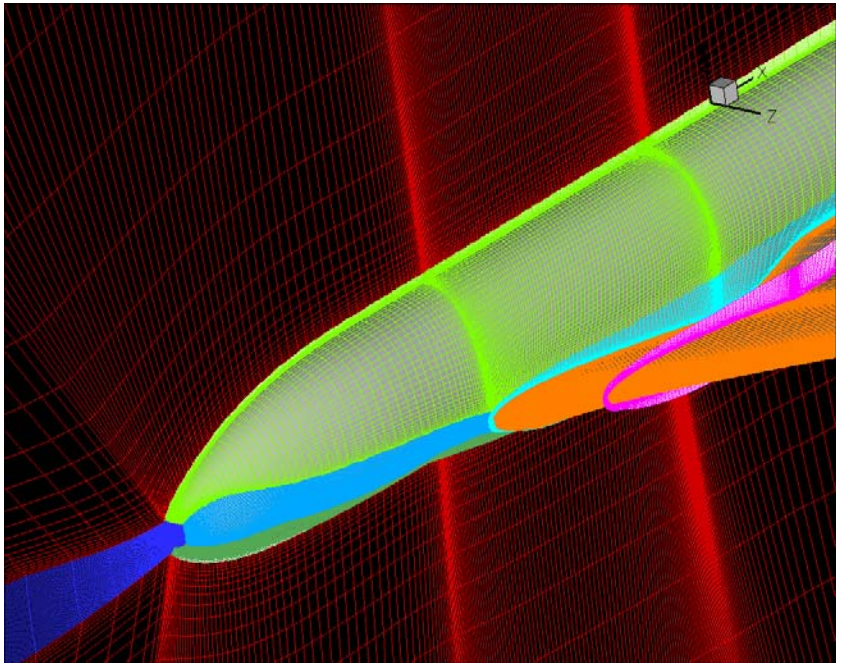

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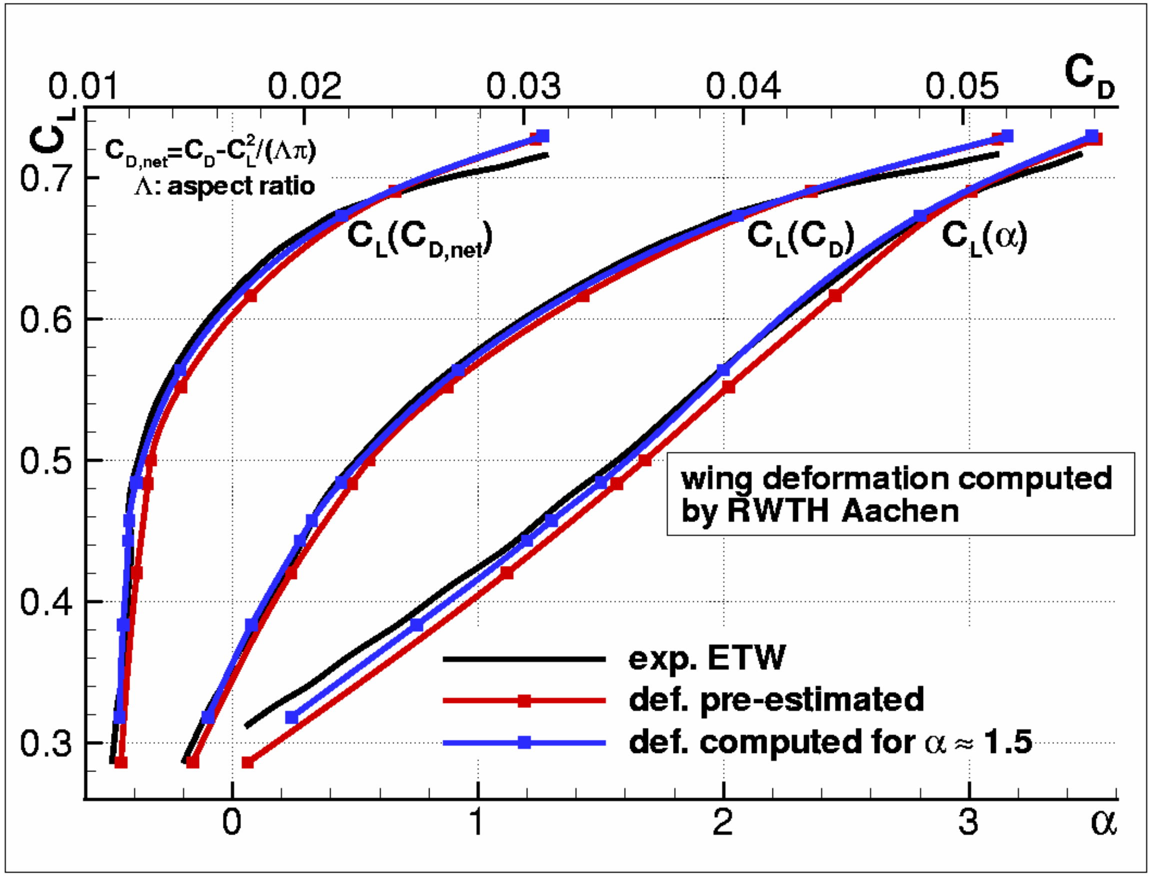

Aerodynamic Shape Optimization

Requirements

- complex configurations
- compressible Navier-Stokes equations
  with accurate models for turbulence and transition
- validated and efficient CFD codes
- multi-point design, multi-objective optimization, MDO
- large number of design variables
- physical and geometrical constraints
- meshing & mesh deformation techniques ensuring grid quality
- efficient optimization algorithms
- automatic framework
- parameterization based on CAD model

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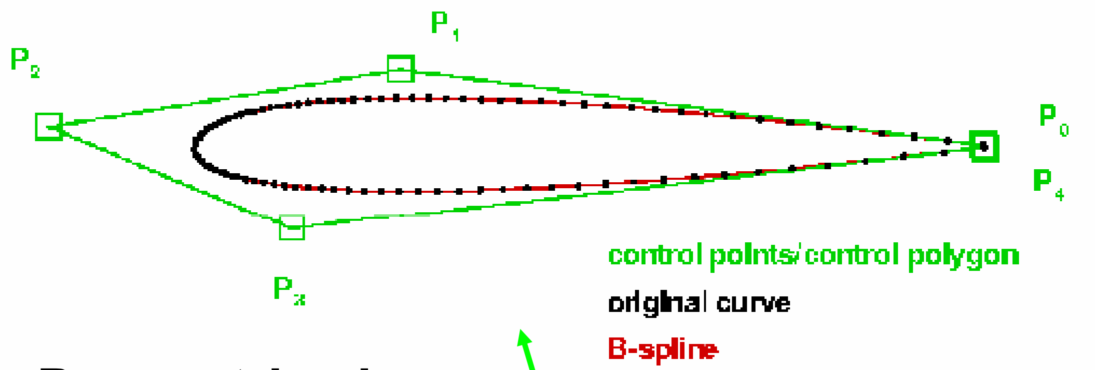
⇓

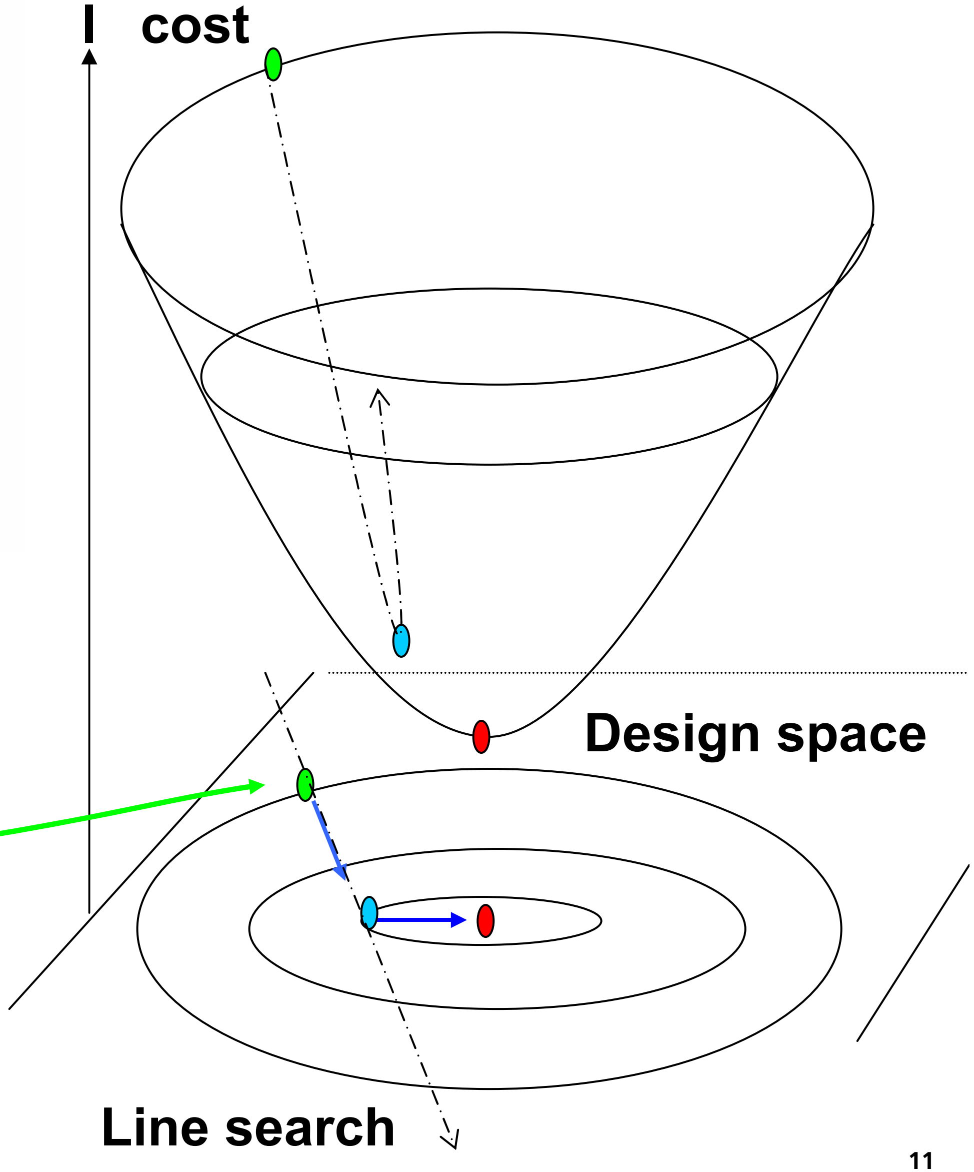
⇒ **Sensitivity based deterministic optimization strategies !!!**

⇒

Aerodynamic Shape Optimization



Parametrized airfoil



Search direction

“ ↘ “ : $-\nabla I = -\left(\dots, \frac{\delta I}{\delta P_i}, \dots\right)^T_{i=1,\dots,n}$

Governing Equations and Aerodynamic Coefficients

Compressible 2D Euler-Equations

$$\frac{\partial w}{\partial t}+\frac{\partial f}{\partial x}+\frac{\partial g}{\partial y}=0$$

while

$$w=\begin{pmatrix}\rho\\ \rho u\\ \rho v\\ \rho E\end{pmatrix}\quad,\quad f=\begin{pmatrix}\rho u\\ \rho u^2+p\\ \rho uv\\ \rho uH\end{pmatrix}\quad,\quad g=\begin{pmatrix}\rho v\\ \rho vu\\ \rho v^2+p\\ \rho vH\end{pmatrix}$$

Pressure (ideal gas)

$$p=(\gamma-1)\rho(E-\frac{1}{2}\vec{v}^2)$$

Dimensionless pressure

$$C_p=\frac{2(p-p_\infty)}{\gamma M_\infty^2 p_\infty}$$

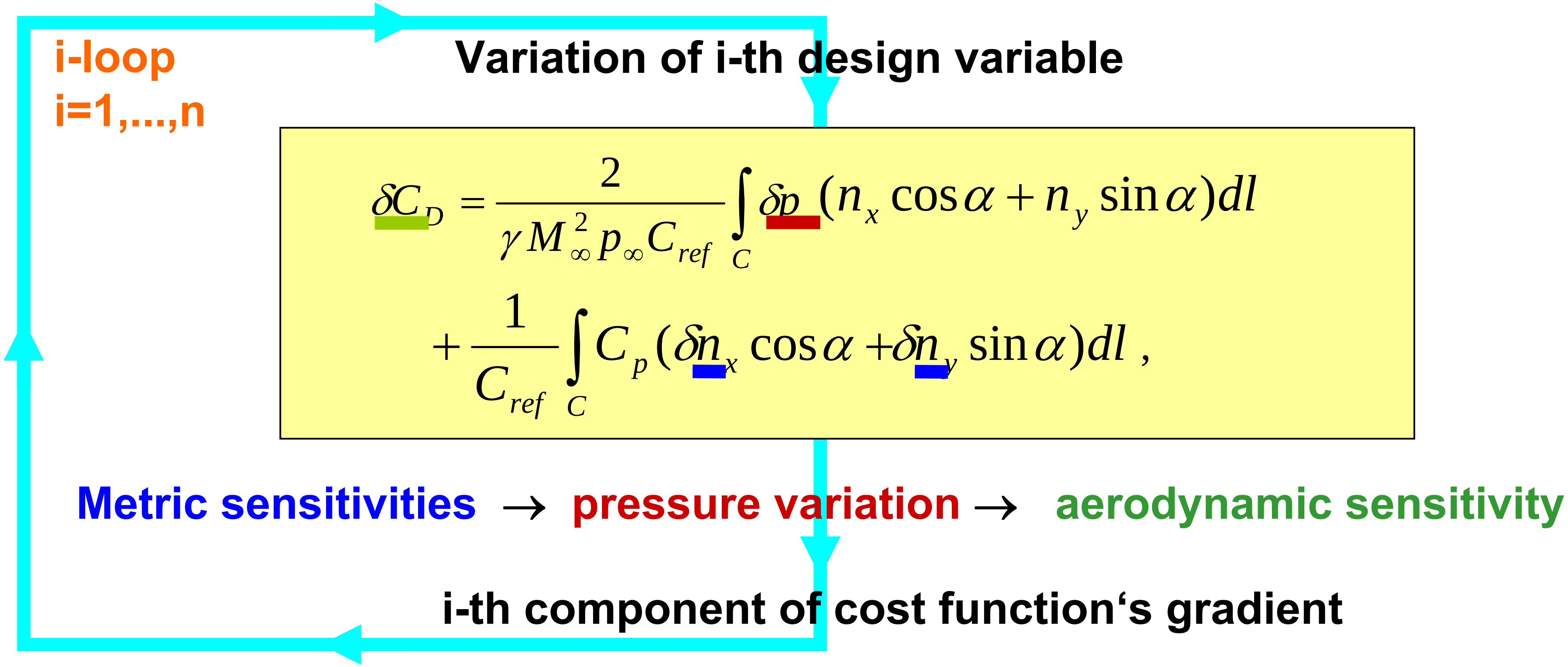
Drag, lift, pitching moment coefficients

$$C_D=\frac{1}{C_{ref}}\int_C C_p(n_x\cos\alpha+n_y\sin\alpha)dl$$

$$C_L=\frac{1}{C_{ref}}\int_C C_p(n_y\cos\alpha-n_x\sin\alpha)dl$$

$$C_m=\frac{1}{C_{ref}^2}\int_C C_p(n_y(x-x_m)-n_x(y-y_m))dl$$

Finite Differences



i-loop
i=1,...,n

Variation of i-th design variable

$$\delta C_D = \frac{2}{\gamma M_\infty^2 p_\infty C_{ref}} \int_C \delta p \,(n_x \cos\alpha + n_y \sin\alpha)\, dl + \frac{1}{C_{ref}} \int_C C_p (\delta n_x \cos\alpha + \delta n_y \sin\alpha)\, dl \;,$$

Metric sensitivities $\rightarrow$ **pressure variation** $\rightarrow$ **aerodynamic sensitivity**

i-th component of cost function‘s gradient

- **Finite Differences** → **n design variables require n+1 flow calculations**

Motivation of Adjoint Approach

High number of design variables

- **Finite Differences** → **n design variables require n+1 flow calculations**

- **Adjoint Approach** → **n design variables require 1 flow and 1 adjoint flow calculation**

  Independent of number of design variables

  High accuracy

Dual or Adjoint (Linear) Problem

Let be $A \in \mathrm{R}^{n\times m}$, $h \in \mathrm{R}^{m}$, $\varphi \in \mathrm{R}^{m}$ and $b \in \mathrm{R}^{n}$.

We define the primal lineare problem:

$$\begin{aligned} \text{evaluate } I &= h^T\varphi\,, && (1)\\ \text{while } A\varphi &= b. && (2)\end{aligned}$$

Furthermore, $\psi \in \mathbb{R}^n$ fulfills:

$$A^T\psi = h. \tag{3}$$

Then eqs. (2) and (3) imply

$$h^T\varphi = (A^T\psi)^T\varphi = (A^T\psi, \varphi) = (\psi, A\varphi) = \psi^T A\varphi = \psi^T b \quad \forall\varphi, \psi \tag{4}$$

and we have the equivalent dual or adjoint linear problem:

$$\begin{aligned} \text{evaluate } I &= \psi^T b\,, && (5)\\ \text{while } A^T\psi &= h\,. && (6)\end{aligned}$$

The vector $\psi = (\psi_i)_{i\in\{1,\dots,n\}}$ is called the vector of adjoint variables ψ_i.

Continuous Adjoint

We define now the scalar product

$$(h, \varphi) := \int_{\Omega} h^T \varphi dx \ . \tag{7}$$

Let φ be the solution of the PDE

$$L\varphi = b \tag{8}$$

in the domain Ω, which fulfills the homogeneous boundary conditions on $\partial\Omega$.

Then L^*, the dual or adjoint operator of L, is defined as:

$$L^* : \quad (\psi, L\varphi) = (L^*\psi, \varphi) \quad \forall \varphi, \psi. \tag{9}$$

Furthermore, ψ, the vector(-field) of adjoint variables, solves the dual or adjoint PDE

$$L^*\psi = h \tag{10}$$

in the domain Ω and again fulfills the homogeneous boundary conditions on $\partial\Omega$.

Then finally we have as before:

$$(h, \varphi) = (L^*\psi, \varphi) = (\psi, L\varphi) = (\psi, b). \tag{11}$$

Examples of Adjoint Operators

Let's take e.g. the convection-diffusion equation

$$L\varphi \equiv \frac{d\varphi}{dx} - \epsilon\frac{d^2\varphi}{dx^2}, \quad 0 < x < 1, \tag{12}$$

with homogeneous boundary conditions $\varphi(0) = \varphi(1) = 0$.

Integration by parts yields ($\varphi, \psi \in \mathcal{C}^2$):

$$\begin{aligned}
(\psi, L\varphi) &= \int_0^1 \psi\left(\frac{d\varphi}{dx} - \epsilon\frac{d^2\varphi}{dx^2}\right)\,dx && (13)\\
&= \int_0^1 \left(-\frac{d\psi}{dx} - \epsilon\frac{d^2\psi}{dx^2}\right)\varphi\,dx + \left[\psi\varphi - \epsilon\psi\frac{d\varphi}{dx} + \epsilon\varphi\frac{d\psi}{dx}\right]_0^1 && (14)\\
&= \int_0^1 \underbrace{\left(-\frac{d\psi}{dx} - \epsilon\frac{d^2\psi}{dx^2}\right)}_{=:L^*\psi}\varphi\,dx + \left[-\epsilon\psi\frac{d\varphi}{dx}\right]_0^1. && (15)
\end{aligned}$$

Examples of Adjoint Operators

For the adjoint convection-diffusion equation

$$L^*\psi \equiv -\frac{d\psi}{dx} - \epsilon\frac{d^2\psi}{dx^2}, \tag{16}$$

with homogeneous boundary conditions $\psi(0) = \psi(1) = 0$, the boundary term (15) vanishes and it holds (11):

$$(h, \varphi) = (L^*\psi, \varphi) = (\psi, L\varphi) = (\psi, b).$$

Some examples:

	Operator	**Adjoint**
Convection-Diffusion Eq.	$\frac{d\varphi}{dx} - \epsilon\frac{d^2\varphi}{dx^2}$	$-\frac{d\psi}{dx} - \epsilon\frac{d^2\psi}{dx^2}$
Wave Eq.	$\frac{d\varphi}{dt} - \frac{d^2\varphi}{dx^2}$	$-\frac{d\psi}{dt} - \frac{d^2\psi}{dx^2}$
Convection Eq.	$\frac{d\varphi}{dt} + \frac{d\varphi}{dx}$	$-\frac{d\psi}{dt} - \frac{d\psi}{dx}$

How to get the gradient using adjoint theory

Let the optimization problem be stated as

$$\min_{D} I(W, X, D),$$

and with the governing equations

$$R(W, X, D) = 0$$

with W the flow variables, X the mesh and D the design variables.

We introduce the Lagrangian multiplyer Λ and define the Lagrangian L as

$$L = I + \Lambda^T R$$

How to get the gradient using adjoint theory

The derivatives of *L* with respect to the design variables *D* are:

$$\frac{dL}{dD} = \frac{d}{dD}\left(I\left(W, X, D\right) + \Lambda^T R\left(W, X, D\right)\right)$$

How to get the gradient using adjoint theory

The derivatives of *L* with respect to the design variables *D* are:

$$\begin{aligned}\frac{dL}{dD} &= \frac{d}{dD}\left(I\left(W,X,D\right)+\Lambda^{T}R\left(W,X,D\right)\right)\\ &= \left\{\frac{\partial I}{\partial W}\frac{dW}{dD}+\frac{\partial I}{\partial X}\frac{dX}{dD}+\frac{\partial I}{\partial D}\right\}+\Lambda^{T}\left\{\frac{\partial R}{\partial W}\frac{dW}{dD}+\frac{\partial R}{\partial X}\frac{dX}{dD}+\frac{\partial R}{\partial D}\right\}\end{aligned}$$

How to get the gradient using adjoint theory

The derivatives of *L* with respect to the design variables *D* are:

$$
\begin{aligned}
\frac{dL}{dD} &= \frac{d}{dD}\left(I\left(W, X, D\right) + \Lambda^T R\left(W, X, D\right)\right) \\
&= \left\{\frac{\partial I}{\partial W}\frac{dW}{dD} + \frac{\partial I}{\partial X}\frac{dX}{dD} + \frac{\partial I}{\partial D}\right\} + \Lambda^T \left\{\frac{\partial R}{\partial W}\frac{dW}{dD} + \frac{\partial R}{\partial X}\frac{dX}{dD} + \frac{\partial R}{\partial D}\right\} \\
&= \left\{\frac{\partial I}{\partial W} + \Lambda^T \frac{\partial R}{\partial W}\right\}\frac{dW}{dD} + \left\{\frac{\partial I}{\partial X} + \Lambda^T \frac{\partial R}{\partial X}\right\}\frac{dX}{dD} + \left\{\frac{\partial I}{\partial D} + \Lambda^T \frac{\partial R}{\partial D}\right\}
\end{aligned}
$$

How to get the gradient using adjoint theory

The derivatives of *L* with respect to *D* are:

$$\begin{aligned}\frac{dL}{dD} &= \left\{\frac{\partial I}{\partial X} + \Lambda^T \frac{\partial R}{\partial X}\right\}\frac{dX}{dD} + \\ &\left\{\frac{\partial I}{\partial D} + \Lambda^T \frac{\partial R}{\partial D}\right\} + \\ &\underbrace{\left\{\frac{\partial I}{\partial W} + \Lambda^T \frac{\partial R}{\partial W}\right\}}_{=0}\enclose{circle}{\frac{dW}{dD}}\end{aligned}$$

Metric sensitivities

→ **relatively inexpensive with finite differences**

Partial variations according to the design variables

→ **relatively inexpensive**

Variations w. r. t. the flow variables

→ **expensive to evaluate**

The expensive component can be canceled by solving the adjoint equation

How to get the gradient using adjoint theory

After solving the adjoint equation,

$$\frac{\partial I}{\partial W} + \Lambda^T \frac{\partial R}{\partial W} = 0$$

the derivatives of *L* with respect to *D* are evaluated according to

$$\frac{dL}{dD} = \left\{ \frac{\partial I}{\partial X} + \Lambda^T \frac{\partial R}{\partial X} \right\} \frac{dX}{dD} + \left\{ \frac{\partial I}{\partial D} + \Lambda^T \frac{\partial R}{\partial D} \right\}$$

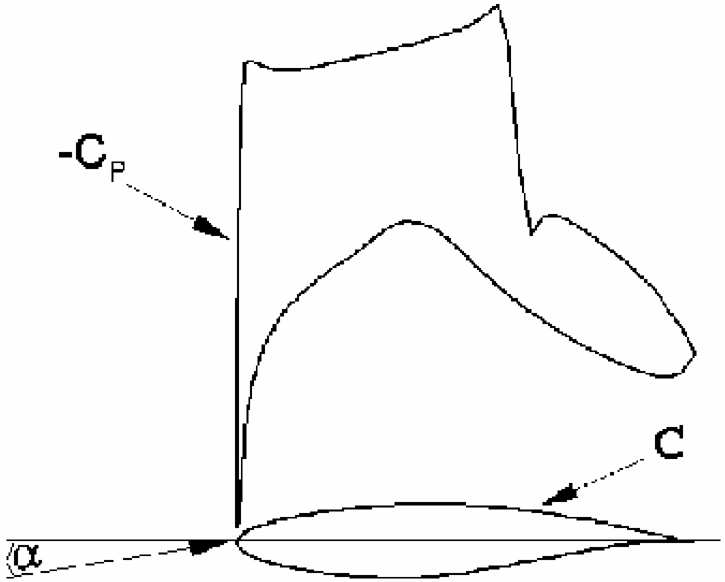
Different Adjoint Approaches

- Continuous Adjoint
  - optimize then discretize
  - hand coded adjoint solvers
  - time consuming in implementation
  - efficient in run and memory

- Discrete Adjoint / Algorithmic Differentiation (AD)
  - discretize then optimize
  - hand coding of adjoint solvers or …
  - … more or less automated generation
  - memory effort increases (way out e.g. check-pointing)

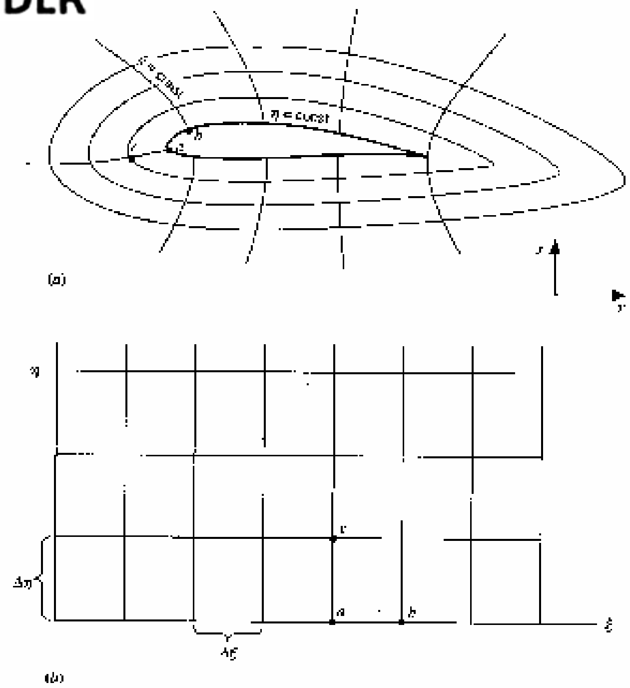
- Hybrid Adjoint
  - use source to source AD tools
  - optimize differentiated code
  - merge “continuous and discrete” routines

Nomenclature



D	flow field domain
B	far field
C	wall
$\partial D := B \cup C$	flow field boundary
$\vec{S} := \binom{S_x}{S_y}$	normal vector $\perp \partial D$
$\vec{n} := \binom{n_1}{n_2}$	normal unit vector $\perp \partial D$
α	angle of attack
C_D	drag coefficient
C_L	lift coefficient
p	pressure
M	Mach number
$)_\infty$	. . . at free stream
γ	ratio of specific heats
S_{ref}	area of airfoil
$\frac{2(p-p_\infty)}{\gamma M_\infty^2 p_\infty} =: C_p$	pressure coefficient

2D Euler Equations in body fitted coordinates



Cartesian coordinates:

$$\frac{\partial w}{\partial t} + \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} = 0$$

$$w = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \end{pmatrix}, f = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ \rho u H \end{pmatrix}, g = \begin{pmatrix} \rho v \\ \rho v u \\ \rho v^2 + p \\ \rho v H \end{pmatrix}$$

$$p = (\gamma - 1)\rho(E - \tfrac{1}{2}(u^2 + v^2)), \qquad \rho H = \rho E + p$$

Body fitted transformation:

$$(x, y) \mapsto (\xi(x, y), \eta(x, y)),$$

$$J = \det \begin{pmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta} \end{pmatrix}, \qquad \begin{pmatrix} U \\ V \end{pmatrix} = \frac{1}{J} \begin{pmatrix} \frac{\partial y}{\partial \eta} & -\frac{\partial x}{\partial \eta} \\ -\frac{\partial y}{\partial \xi} & \frac{\partial x}{\partial \xi} \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}$$

Body fitted coordinates:

$$\frac{\partial W}{\partial t} + \frac{\partial F}{\partial \xi} + \frac{\partial G}{\partial \eta} = 0$$

$$W = J \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \end{pmatrix}, F = J \begin{pmatrix} \rho U \\ \rho U u + \frac{\partial \xi}{\partial x} p \\ \rho U v + \frac{\partial \xi}{\partial y} p \\ \rho U H \end{pmatrix}, G = J \begin{pmatrix} \rho V \\ \rho V u + \frac{\partial \eta}{\partial x} p \\ \rho V v + \frac{\partial \eta}{\partial y} p \\ \rho V H \end{pmatrix}$$

Derivation of the continuous adjoint Euler equations

In the case of steady state it holds for the perturbed geometry

$$\frac{\partial}{\partial \xi}(F + \delta F) + \frac{\partial}{\partial \eta}(G + \delta G) = 0$$

$$\Rightarrow \quad (1) \quad \frac{\partial}{\partial \xi}(\delta F) + \frac{\partial}{\partial \eta}(\delta G) \overset{!}{=} 0.$$

Furthermore

$$(2) \qquad \delta F = \delta\left(J\frac{\partial \xi}{\partial x}\right) f + \delta\left(J\frac{\partial \xi}{\partial y}\right) g + J\frac{\partial \xi}{\partial x}\frac{\partial f}{\partial w}\delta w + J\frac{\partial \xi}{\partial y}\frac{\partial g}{\partial w}\delta w$$

and

$$(3) \qquad \delta G = \delta\left(J\frac{\partial \eta}{\partial x}\right) f + \delta\left(J\frac{\partial \eta}{\partial y}\right) g + J\frac{\partial \eta}{\partial x}\frac{\partial f}{\partial w}\delta w + J\frac{\partial \eta}{\partial y}\frac{\partial g}{\partial w}\delta w.$$

Derivation of the continuous adjoint Euler equations

Together with (1) and the fundamental lemma of variational calculus it holds

$$\int_D \psi^T \left(\frac{\partial}{\partial \xi}(\delta F) + \frac{\partial}{\partial \eta}(\delta G) \right) d\xi d\eta = 0$$

for any Lagrangian multiplier ψ.

If ψ is differentiable one obtains together with Greens formula

$$-\int_D \left(\frac{\partial \psi^T}{\partial \xi} \delta F + \frac{\partial \psi^T}{\partial \eta} \delta G \right) d\xi d\eta + \int_B (n_1 \psi^T \delta F + n_2 \psi^T \delta G) d\xi - \int_C (n_1 \psi^T \delta F + n_2 \psi^T \delta G) d\xi = 0.$$

Derivation of the continuous adjoint Euler equations

Now the variation of the cost function can be expressed as

$$
\begin{aligned}
\delta C_D \;=\;& \frac{2}{\gamma M_\infty^2 p_\infty S_{ref}} \int_C \delta p (S_x \cos\alpha + S_y \sin\alpha)\, d\xi - \int_D \left(\frac{\partial \psi^T}{\partial \xi} \delta F + \frac{\partial \psi^T}{\partial \eta} \delta G \right) d\xi d\eta \\
&+ \int_B (n_1 \psi^T \delta F + n_2 \psi^T \delta G) d\xi - \int_C (\underbrace{n_1 \psi^T \delta F}_{=\,0,\ n_1=0} + n_2 \psi^T \delta G) d\xi \\
&+ \frac{1}{S_{ref}} \int_C C_p (\delta S_x \cos\alpha + \delta S_y \sin\alpha)\, d\xi .
\end{aligned}
$$

Along C it holds $V = 0$ and yields

$$
G = J \begin{pmatrix} 0 \\ \frac{\partial \eta}{\partial x} p \\ \frac{\partial \eta}{\partial y} p \\ 0 \end{pmatrix}, \qquad \delta G = J \begin{pmatrix} 0 \\ \frac{\partial \eta}{\partial x} \delta p \\ \frac{\partial \eta}{\partial y} \delta p \\ 0 \end{pmatrix} + p \begin{pmatrix} 0 \\ \delta \left(J \frac{\partial \eta}{\partial x} \right) \\ \delta \left(J \frac{\partial \eta}{\partial y} \right) \\ 0 \end{pmatrix} .
$$

Derivation of the continuous adjoint Euler equations

Together with (2) and (3) one obtains

$$
\begin{aligned}
\delta C_D = & \frac{2}{\gamma M_\infty^2 p_\infty S_{ref}} \int_C \delta p (S_x \cos\alpha + S_y \sin\alpha)\, d\xi \\
& - \int_D \frac{\partial \psi^T}{\partial \xi} \left(\delta \left(J \frac{\partial \xi}{\partial x} \right) f + \delta \left(J \frac{\partial \xi}{\partial y} \right) g + J \frac{\partial \xi}{\partial x} \frac{\partial f}{\partial w} \delta w + J \frac{\partial \xi}{\partial y} \frac{\partial g}{\partial w} \delta w \right) \\
& \qquad + \frac{\partial \psi^T}{\partial \eta} \left(\delta \left(J \frac{\partial \eta}{\partial x} \right) f + \delta \left(J \frac{\partial \eta}{\partial y} \right) g + J \frac{\partial \eta}{\partial x} \frac{\partial f}{\partial w} \delta w + J \frac{\partial \eta}{\partial y} \frac{\partial g}{\partial w} \delta w \right) d\xi d\eta \\
& - \int_C \psi_2 \left(J \frac{\partial \eta}{\partial x} \delta p + p \delta \left(J \frac{\partial \eta}{\partial x} \right) \right) + \psi_3 \left(J \frac{\partial \eta}{\partial y} \delta p + p \delta \left(J \frac{\partial \eta}{\partial y} \right) \right) d\xi \\
& + \int_B n_1 \psi^T \delta F + n_2 \psi^T \delta G d\xi + \frac{1}{S_{ref}} \int_C C_p (\delta S_x \cos\alpha + \delta S_y \sin\alpha)\, d\xi .
\end{aligned}
$$

If the adjoint Euler equations

$$
\frac{\partial \psi^T}{\partial \xi} \left(J \frac{\partial \xi}{\partial x} \frac{\partial f}{\partial w} + J \frac{\partial \xi}{\partial y} \frac{\partial g}{\partial w} \right) + \frac{\partial \psi^T}{\partial \eta} \left(J \frac{\partial \eta}{\partial x} \frac{\partial f}{\partial w} + J \frac{\partial \eta}{\partial y} \frac{\partial g}{\partial w} \right) = 0 \quad \Leftrightarrow \left(\frac{\partial f}{\partial w} \right)^T \frac{\partial \psi}{\partial x} + \left(\frac{\partial g}{\partial w} \right)^T \frac{\partial \psi}{\partial y} = 0
$$

Derivation of the continuous adjoint Euler equations

... are fulfilled in the domain D with the boundary conditions

$$\frac{2}{\gamma M_\infty^2 p_\infty S_{ref}}(S_x \cos\alpha + S_y \sin\alpha) = \underbrace{-S_x\psi_2 - S_y\psi_3}_{-\frac{\partial y}{\partial \xi}\psi_2 + \frac{\partial x}{\partial \xi}\psi_3 = J\frac{\partial \eta}{\partial x}\psi_2 + J\frac{\partial \eta}{\partial y}\psi_3}$$

on the airfoil C (dependent on the cost function!) and

$$\delta\left(J\frac{\partial \xi}{\partial x}\right), \ldots, \delta\left(J\frac{\partial \eta}{\partial y}\right) \to 0 \qquad \psi^T J \frac{\partial \xi}{\partial x}\frac{\partial f}{\partial w}\delta w = 0, ..., \psi^T J\frac{\partial \eta}{\partial y}\frac{\partial g}{\partial w}\delta w = 0$$

at the far field B one can simplify δC_D to

$$\begin{aligned} \delta C_D \;\; = \;\; & -\int_D \frac{\partial \psi^T}{\partial \xi}\left(\delta\left(\frac{\partial y}{\partial \eta}\right) f - \delta\left(\frac{\partial x}{\partial \eta}\right) g\right) + \frac{\partial \psi^T}{\partial \eta}\left(-\delta\left(\frac{\partial y}{\partial \xi}\right) f + \delta\left(\frac{\partial x}{\partial \xi}\right) g\right) d\xi d\eta \\ & -\int_C p\left(\delta S_x \psi_2 + \delta S_y \psi_3\right) d\xi + \frac{1}{S_{ref}}\int_C C_p(\delta S_x \cos\alpha + \delta S_y \sin\alpha)\, d\xi. \end{aligned}$$

Continuous Adjoint Approach

Adjoint Euler-Equations:

$$-\frac{\partial \psi}{\partial t}-\left(\frac{\partial f}{\partial w}\right)^T\frac{\partial \psi}{\partial x}-\left(\frac{\partial g}{\partial w}\right)^T\frac{\partial \psi}{\partial y}=0$$

Ψ: Vector of adjoint variables

Boundary conditions:

Wall: $n_x\psi_2+n_y\psi_3=\underline{-d(I)}$

Farfield: $\delta x_\xi,\ldots,\delta y_\eta=0,\;\delta w=0$

Adjoint volume formulation of cost function's gradient:

$$\delta I=-\int_C p(-\psi_2\delta y_\xi+\psi_3\delta x_\xi)dl+\underline{K(I)}$$

$$-\int_D \psi_\xi^T(\delta y_\eta f-\delta x_\eta g)+\psi_\eta^T(-\delta y_\xi f+\delta x_\xi g)dA$$

Continuous Adjoint Approach

$$d(C_D) = \frac{2}{\gamma M_\infty^2 p_\infty C_{ref}}(n_x \cos\alpha + n_y \sin\alpha)$$

Drag

$$K(C_D) = \frac{1}{C_{ref}} \int_C C_p (\delta n_x \cos\alpha + \delta n_y \sin\alpha) dl$$

$$d(C_L) = \frac{2}{\gamma M_\infty^2 p_\infty C_{ref}}(n_y \cos\alpha - n_x \sin\alpha)$$

Lift

$$K(C_L) = \frac{1}{C_{ref}} \int_C C_p (\delta n_y \cos\alpha - \delta n_x \sin\alpha) dl$$

$$d(C_m) = \frac{2}{\gamma M_\infty^2 p_\infty C_{ref}^2}(n_y (x - x_m) - n_x (y - y_m))$$

Pitching moment

$$K(C_m) = \frac{1}{C_{ref}^2} \int_C C_p \delta(n_y (x - x_m) - n_x (y - y_m)) dl$$

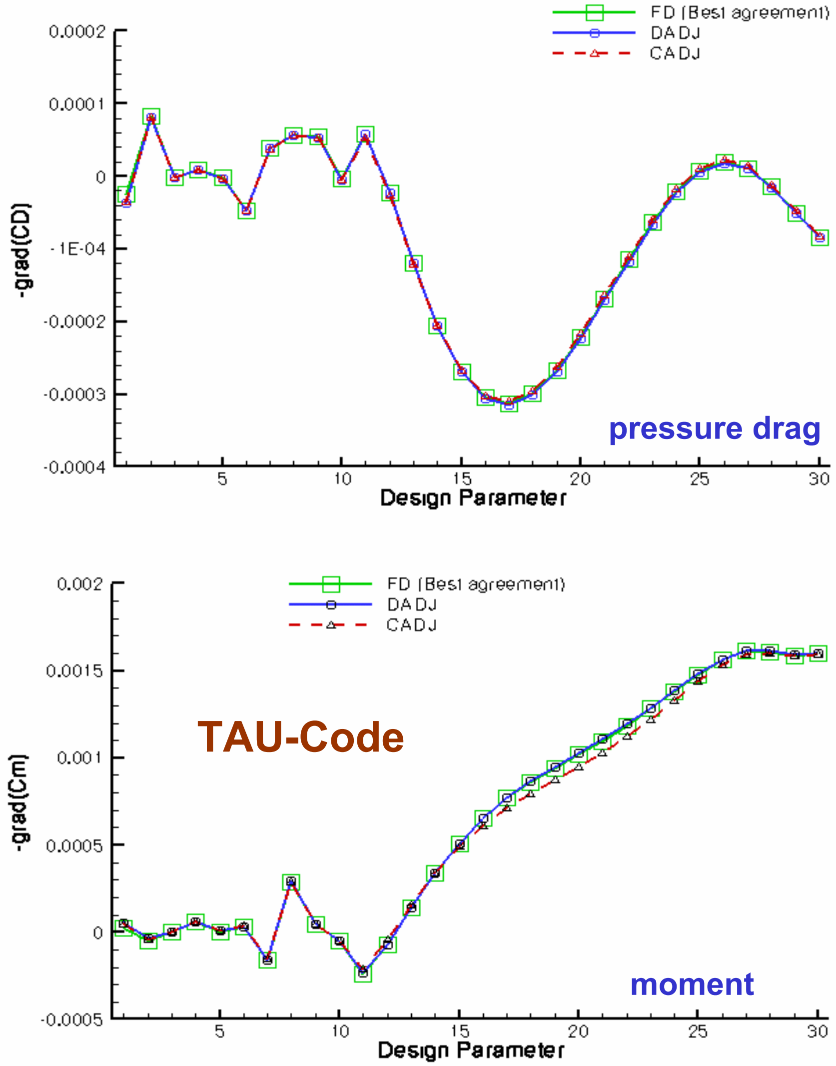
Adjoint solvers

Continuous adjoint

- Euler implemented in FLOWer & TAU
- surface formulation for gradient evaluation
- one shot method (FLOWer)
- coupled aero-structure adjoint (FLOWer)
- Navier-Stokes (frozen μ) implemented in FLOWer, robustness problems

Discrete adjoint

- implemented in TAU
- Euler & RANS with several turbulence models
- currently high memory requirements
- experience with automatic differentiation (FLOWer and TAUij)

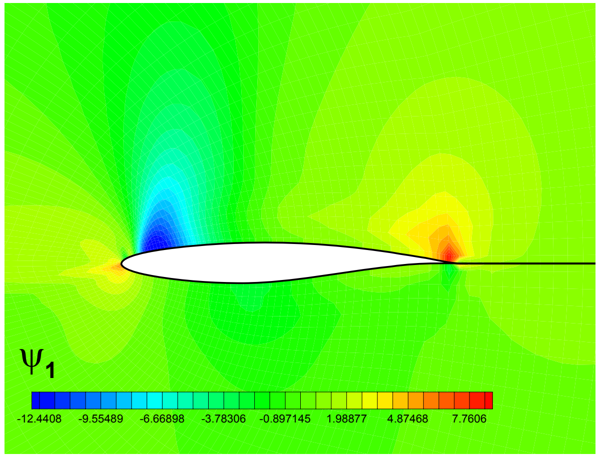


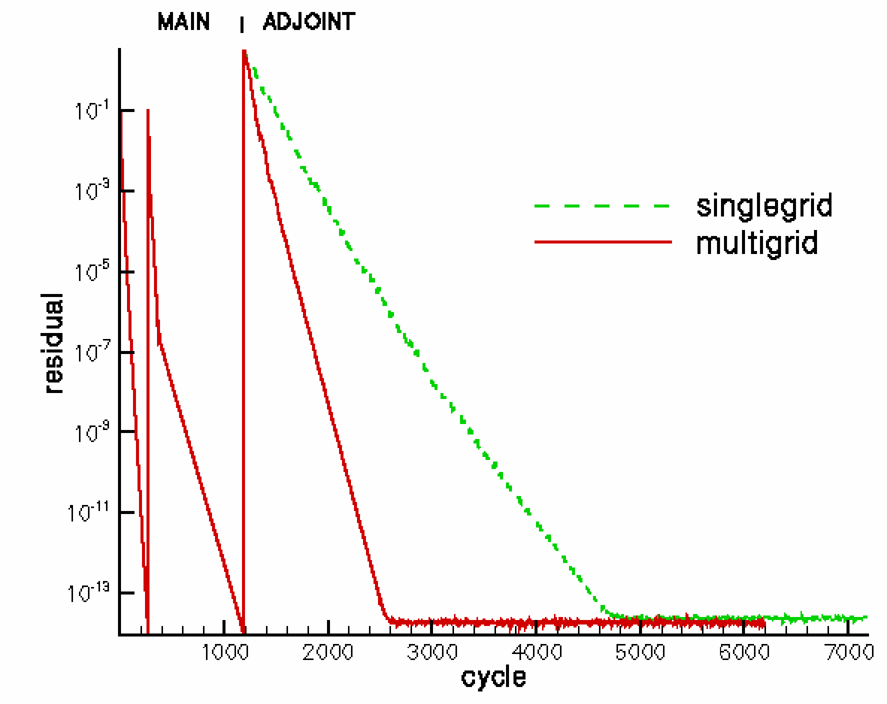
comparison of gradients (airfoil, inviscid)

Continuous adjoint solver FLOWer

Adjoint solver on block-structured grids

- **continuous adjoint approach**
- **implemented in FLOWer**
- **cost functions: lift, drag & moment and combinations**
- **adjoint solver based on multigrid**
- **Euler & Navier-Stokes (frozen μ)**





convergence history, FLOWer

Validation of continuous adjoint solver in FLOWer

Adjoint approach vs. finite differences‘ gradient

finite differences:

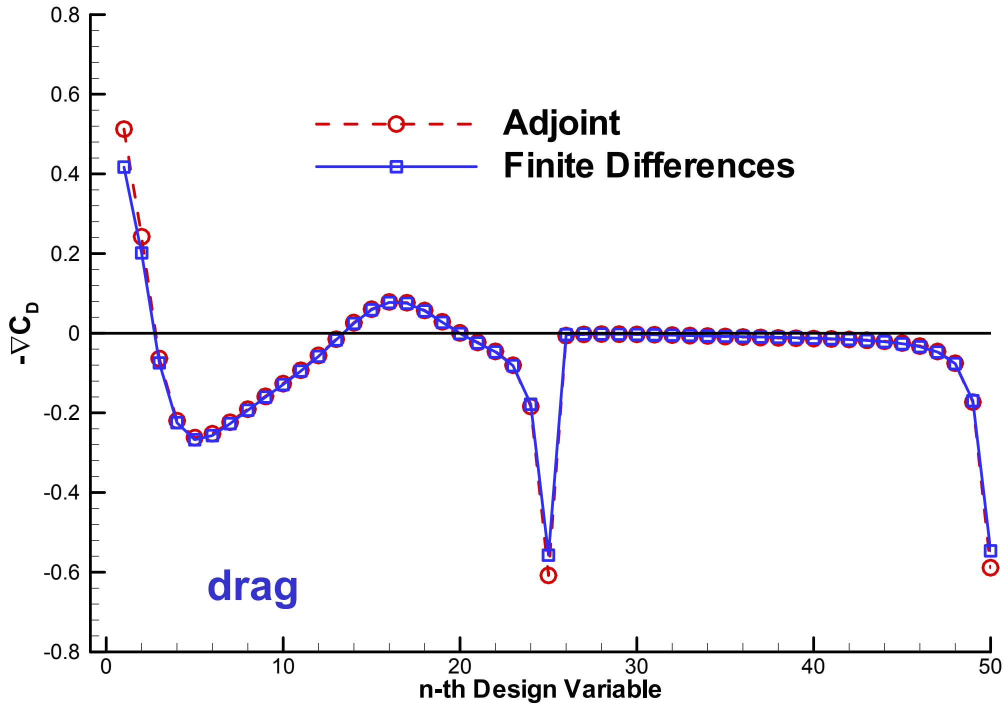
51 calls of FLOWer MAIN

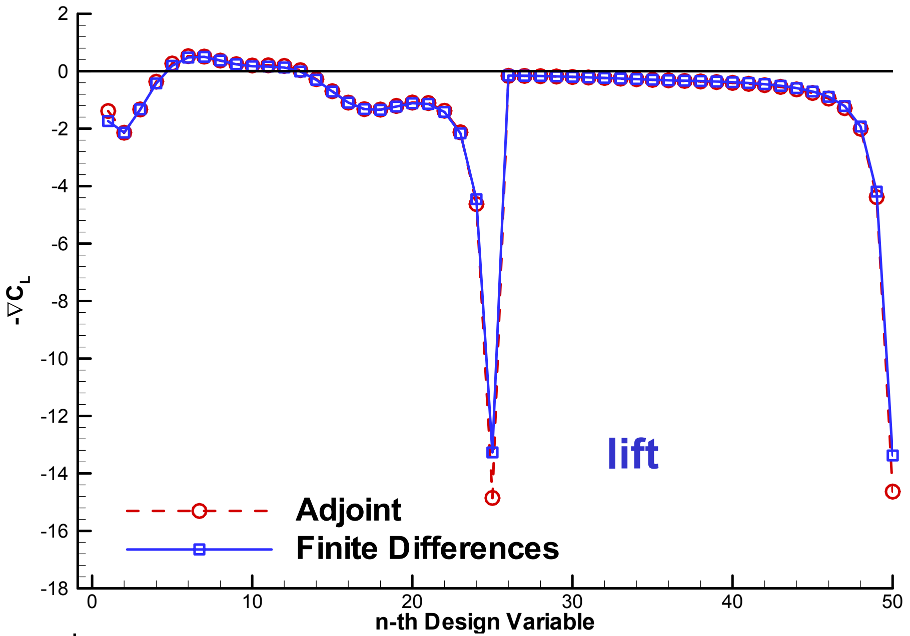
adjoint approach:

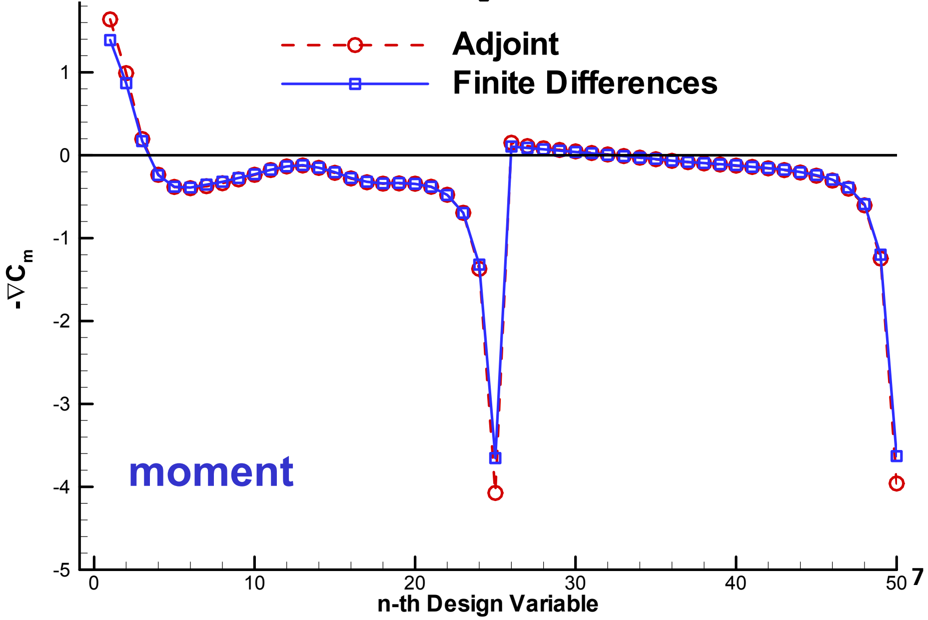
1 call of FLOWer MAIN

3 calls of FLOWer ADJOINT

RAE2822
M_∞=0.73, $\alpha = 2.0°$
50 design variables
(B-spline)







Validation of adjoint gradient based optimization

Objective function

- Drag reduction for RAE 2822 airfoil
- M_∞ =0.73, α=2.00°

Constraints

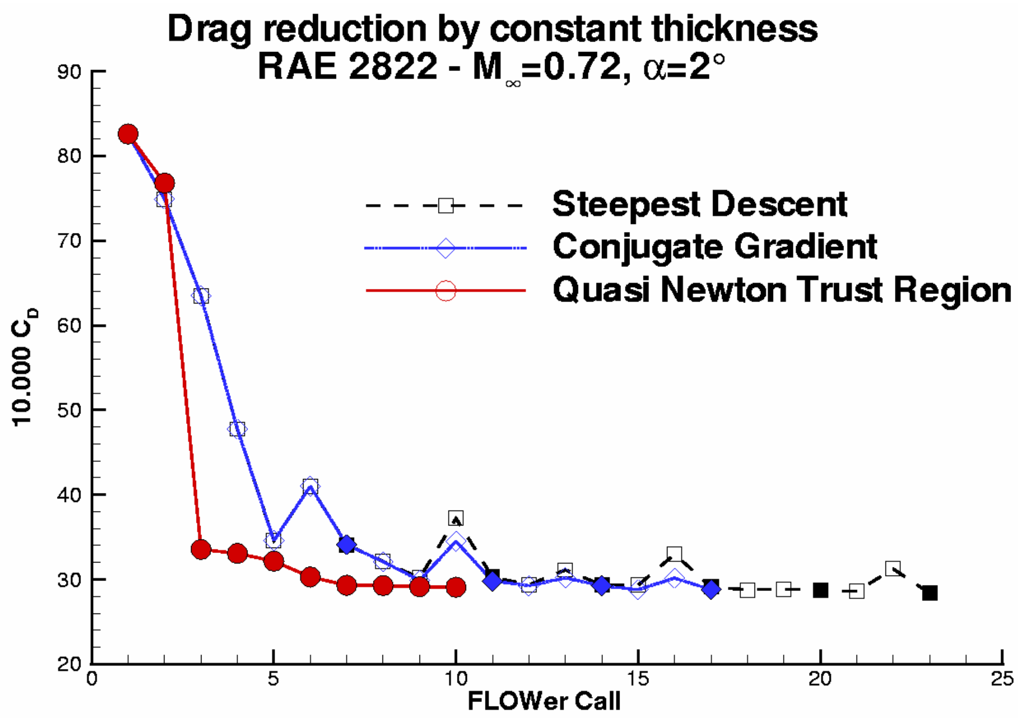
- Constant thickness

Approach

- FLOWer Euler Adjoint
- Deformation of camberline (20 Hicks-Henne functions)

Optimizer

- Steepest Descent
- Conjugate Gradient
- Quasi Newton Trust Region



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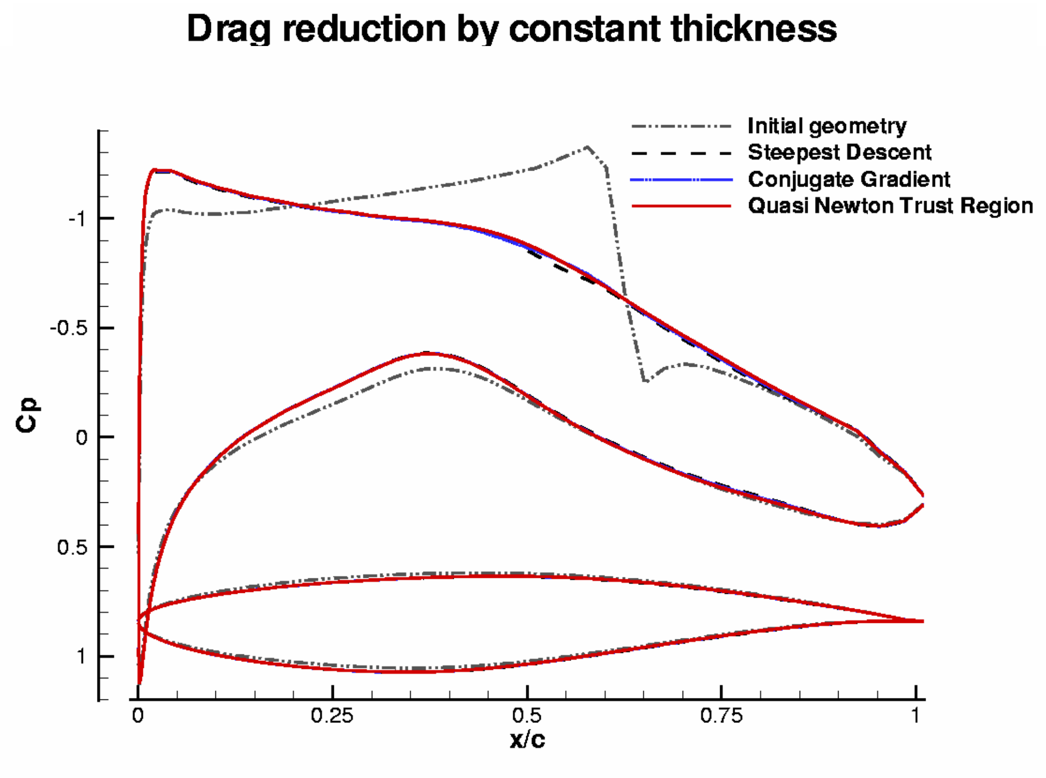
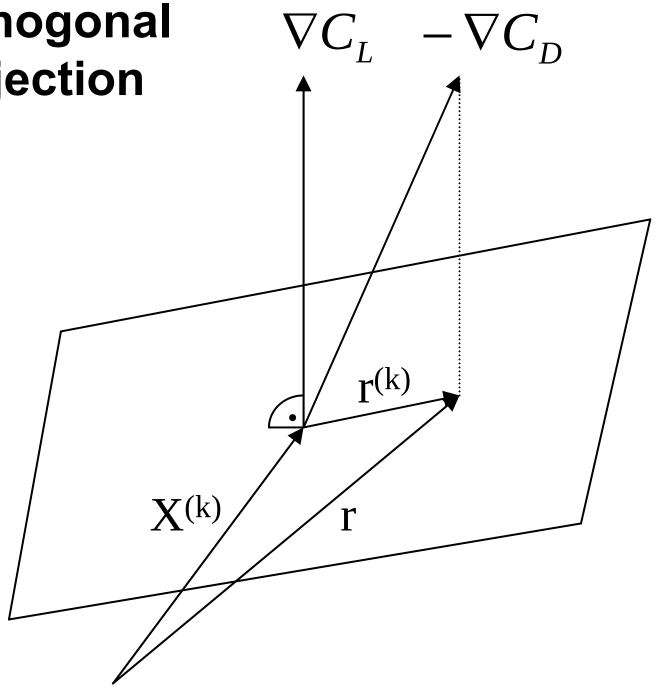


Treatment of Constraints

Orthogonal projection



In direction $r^{(k)}$ the drag is reduced while the lift is held constant

$$\frac{dC_L(X^{(k)})}{dr^{(k)}} = (\nabla_{X^{(k)}} C_L)^T \frac{r^{(k)}}{\left\| r^{(k)} \right\|} = 0$$

$$C_L(r) \approx C_L(X^{(k)})$$

Schmidt - orthogonalization

$$\{a_1, a_2, a_3\} = \{\nabla C_L, \nabla C_m, -\nabla C_D\}$$

$$\downarrow$$

$$\{b_1, b_2, b_3\}:$$

$$\begin{cases} b_1 = a_1\,, \\ b_{l+1} = a_{l+1} - \sum_{i=1}^{l} \frac{b_i^T a_{l+1}}{\left\| b_i \right\|^2} b_i \quad l = 1,2\,. \end{cases}$$

it holds

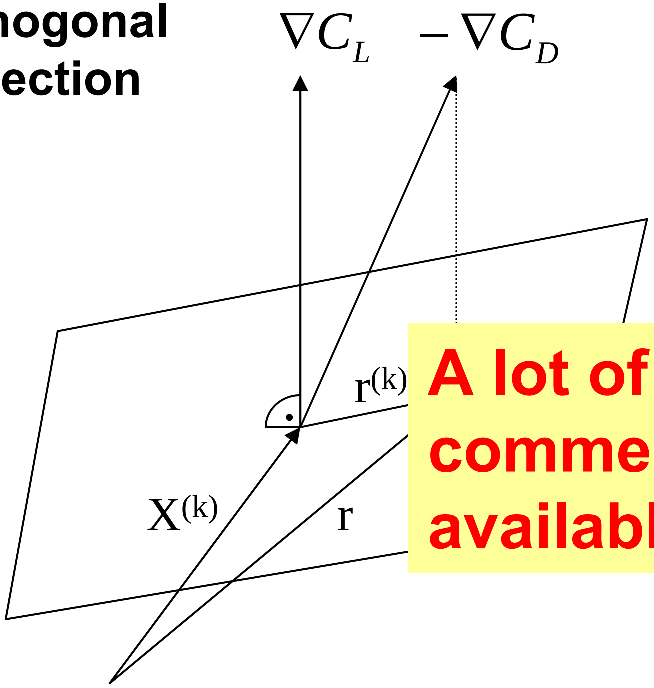
$$a_i^T b_3 = 0\,, \quad i = 1,2$$

$$b_3 = -\nabla C_D + \sum_{i=1}^{2} \frac{b_i^T \nabla C_D}{\left\| b_i \right\|^2} b_i$$

In direction b_3 the drag is reduced while the lift and pitching moment are held constant

Treatment of Constraints

Orthogonal projection



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$$b_{l+1} = a_{l+1} - \sum_{i=1} \frac{b_i \; a_{l+1}}{\|b_i\|^2} b_i \quad l = 1,2 .$$

it holds $a_i^T b_3 = 0 , \quad i = 1,2$

$$b_3 = -\nabla C_D + \sum_{i=1}^{2} \frac{b_i^T \nabla C_D}{\|b_i\|^2} b_i$$

In direction b_3 the drag is reduced while the lift and pitching moment are held constant

A lot of other strategies and commercial packages are available !!!

Multi-constraint airfoil optimization RAE2822

Objective function

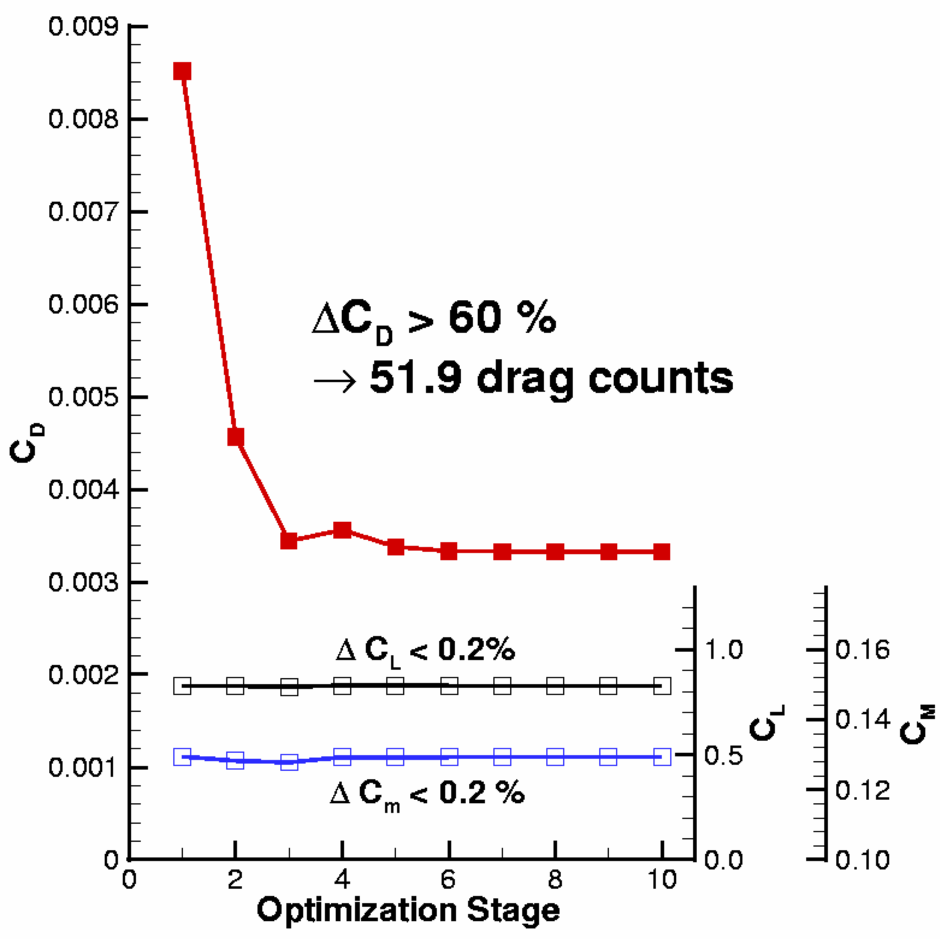
- Drag reduction for RAE 2822 airfoil
- $M_\infty = 0.73$, $\alpha = 2.0°$

Constraints

- Lift, pitching moment and angle of attack held constant
- Constant thickness

Approach

- FLOWer Euler Adjoint
- Constraints handled by feasible direction
- Deformation of camberline



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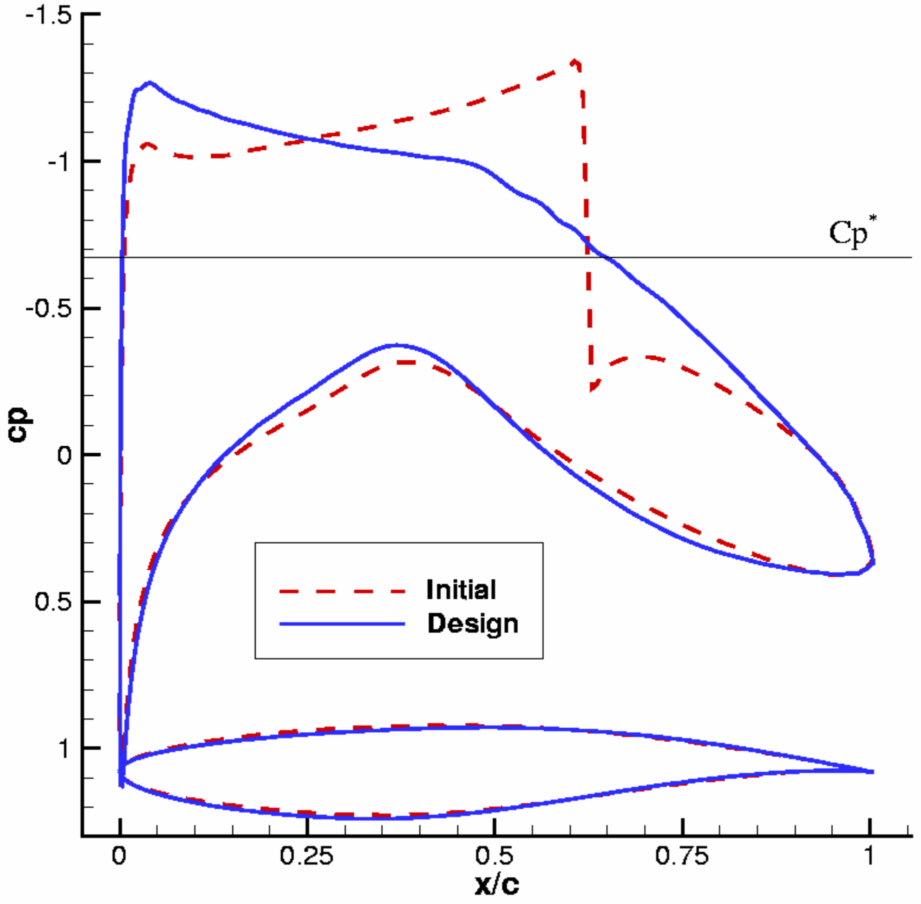


surface pressure distribution

Multipoint airfoil optimization RAE2822

$$I = \sum_{i=1}^{2} W_i C_d(\alpha_i, M_i)$$

Objective function

- Reduction of drag in 2 design points

Design points

- 1 : M_∞=0.734, CL = 0.80 , α = 2.8°, Re=6.5x10^6, xtrans=3%, W_1=2
- 2 : M_∞=0.754, CL = 0.74 , α = 2.8°, Re=6.2x10^6, xtrans=3%, W_2=1

Constraints

- No lift decrease, no change in angle of incidence
- Variation in pitching moment less than 2% in each point
- Maximal thickness constant and at 5% chord more than 96% of initial
- Leading edge radius more than 90% of initial
- Trailing edge angle more than 80% of initial

Multipoint airfoil optimization RAE2822

Parameterization

- 20 design variables changing camberline, Hicks-Henne functions

Optimization strategy

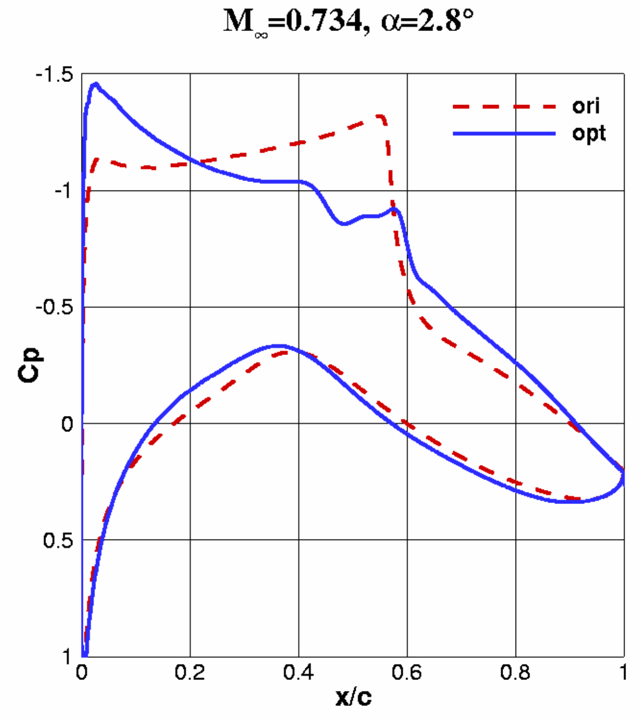
- Constrained SQP
- Navier-Stokes solver FLOWer, Baldwin/Lomax turbulence model
- Gradients provided by FLOWer Adjoint, based on Euler equations

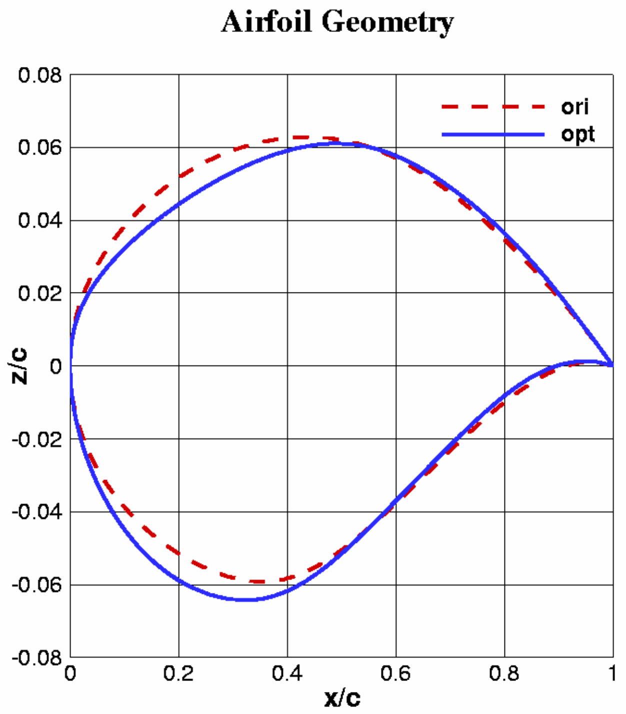
Results

Pt	α	M_i	cl^t	cd^t $(.10^{-4})$	cl	cd^t $(.10^{-4})$	$\Delta cd/cd^t$	$\Delta cl/cl^t$	$\Delta cm/cm^t$
1	2.8	0.734	0.811	197.1	0.811	135.5	-31.2%	0%	+1.6%
2	2.8	0.754	0.806	300.8	0.828	215.0	-27.4%	+2.7%	+2.0%

Multipoint airfoil optimization RAE2822

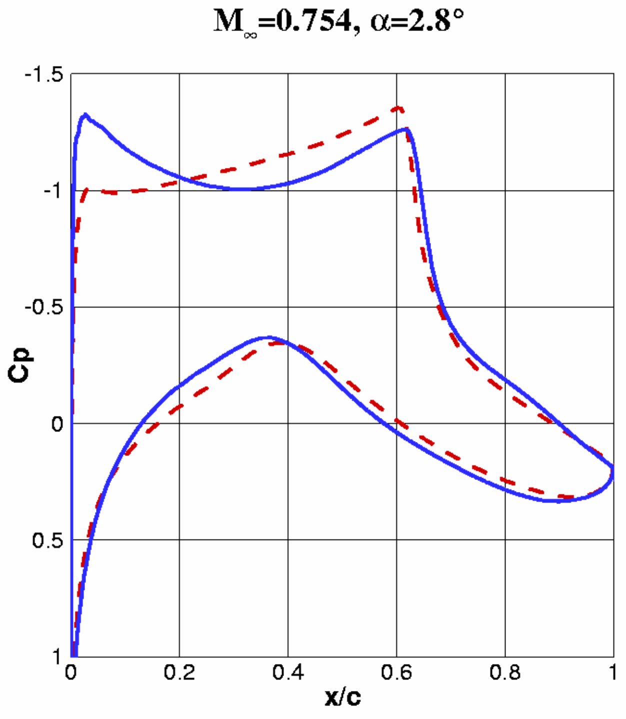
1. design point



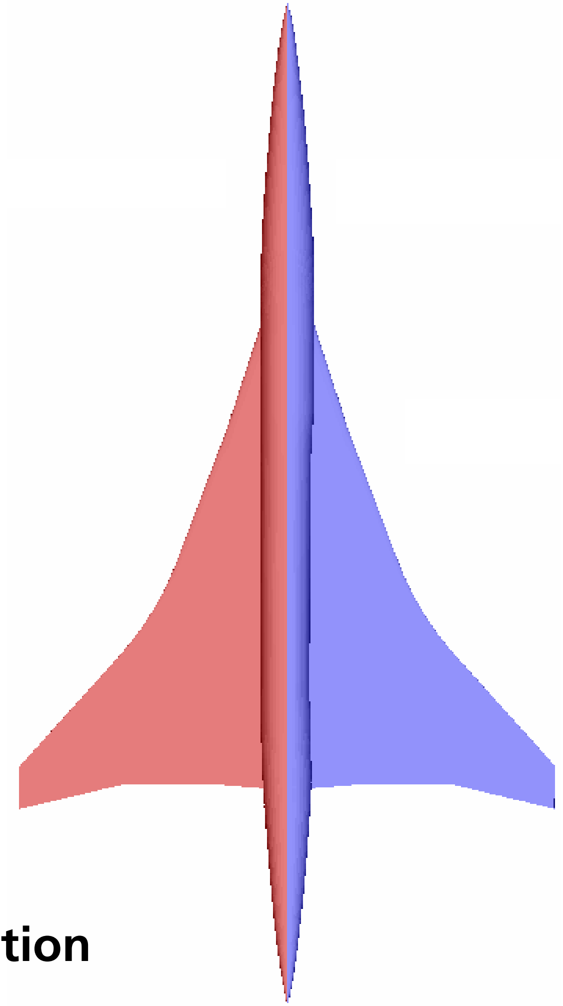


shape geometry

2. design point



Optimization of SCT Configuration
(SCT – Supersonic Cruise Transporter)



Objective function

- drag reduction by constant lift

Design point

- Mach number = 2.0
- lift coefficient = 0.12

Constraints

- fuselage incidence
- minimum fuselage radius
- wing planform unchanged
- minimum wing thickness distribution in spanwise direction

Optimization of SCT Configuration

Approach

- FLOWer code in Euler mode with target lift option
- Lift kept constant by adjusting angle of attack
- FLOWer code in Euler adjoint mode
- Adjoint gradient formulation
- Structured mono-block grid (MegaCads), 230.000 grid points

Optimization strategy

- Quasi-Newton Method (BFGS algorithm)

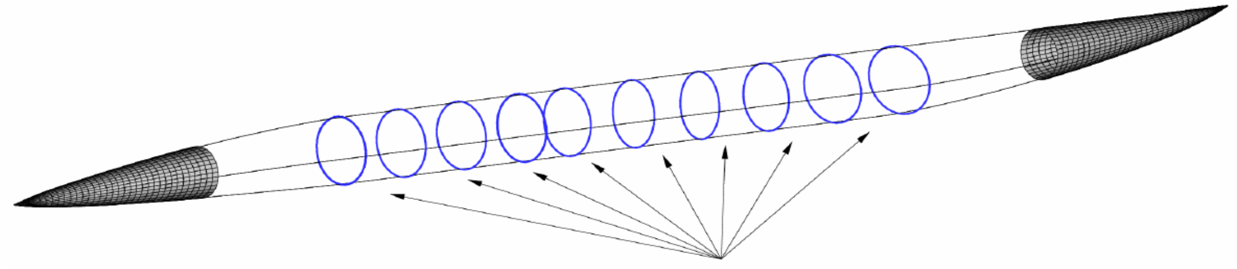
Optimization of SCT Configuration

Design variables

- fuselage: 10 parameters
- twist deformation: 10 parameters
- camberline (8 sections): 32 parameters
- thickness (8 sections): 32 parameters
- angle of attack: 1 parameter

85 parameters

Fuselage



10 sections controlled by Bezier nodes

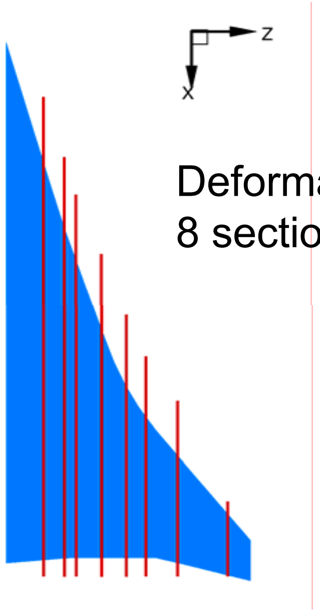
Optimization of SCT Configuration

Design variables

- **fuselage: 10 parameters**
- **twist deformation: 10 parameters**
- **camberline (8 sections): 32 parameters**
- **thickness (8 sections): 32 parameters**
- **angle of attack: 1 parameter**

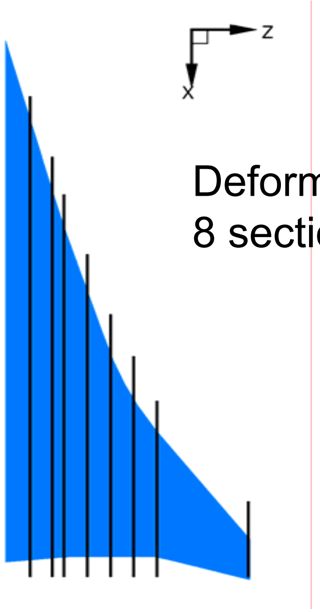
85 parameters

Camberline



Deformation in
8 sections

Thickness



Deformation in
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Optimization of SCT Configuration

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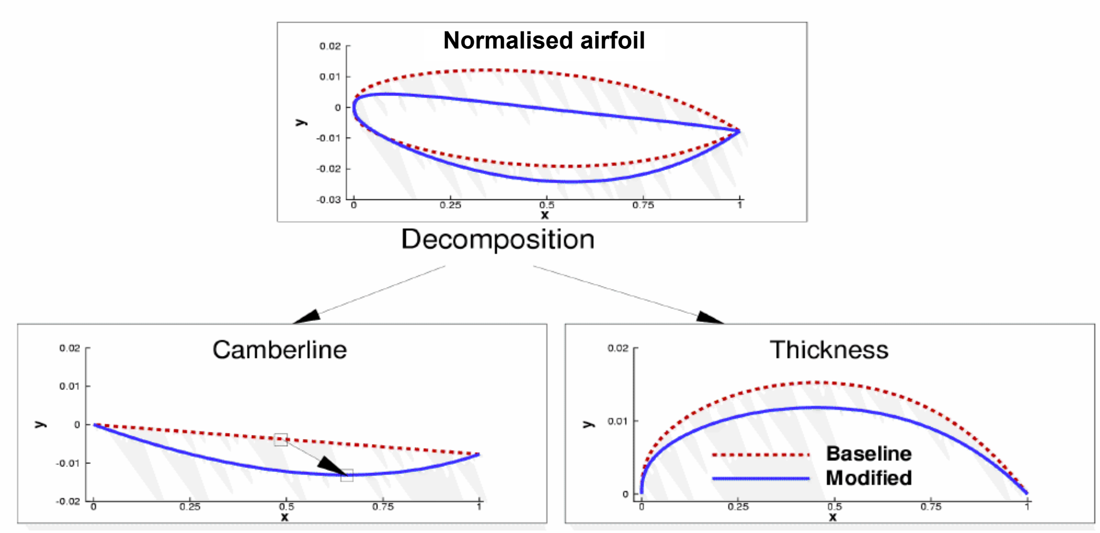
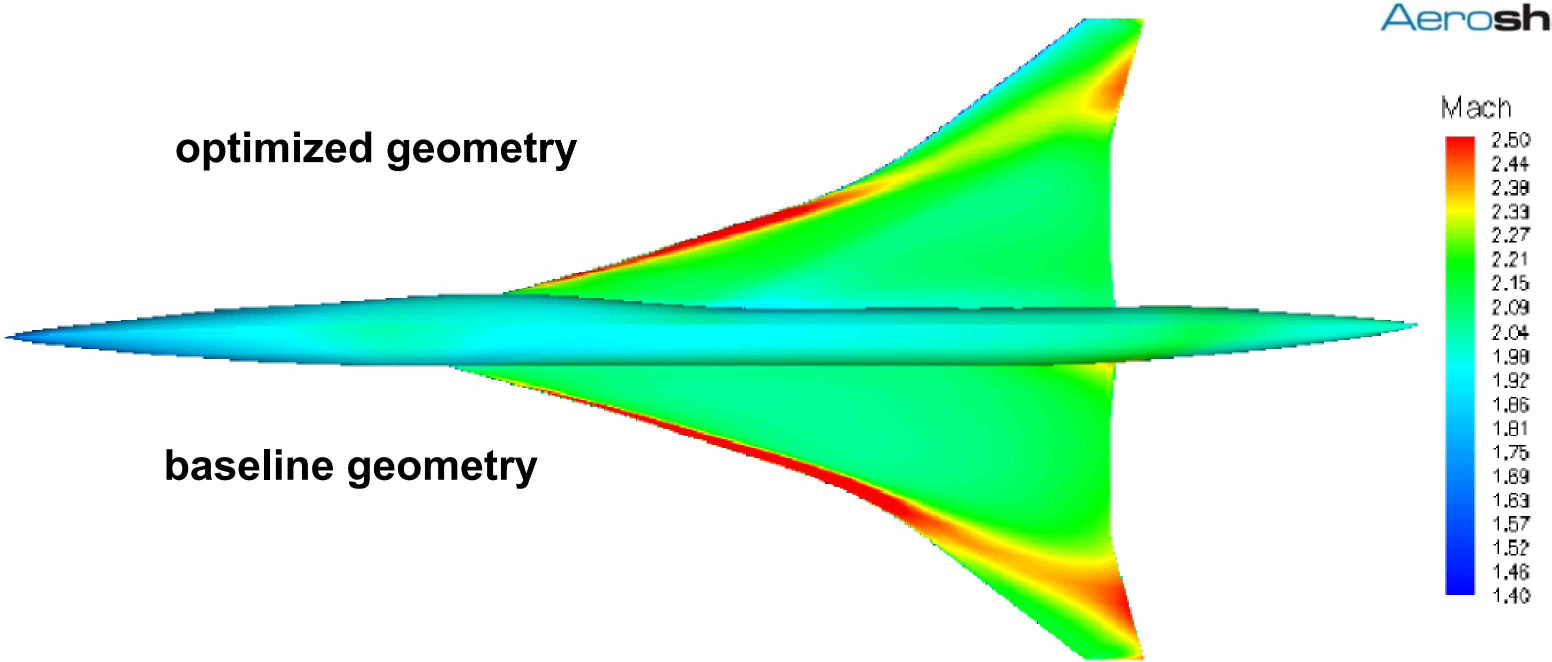
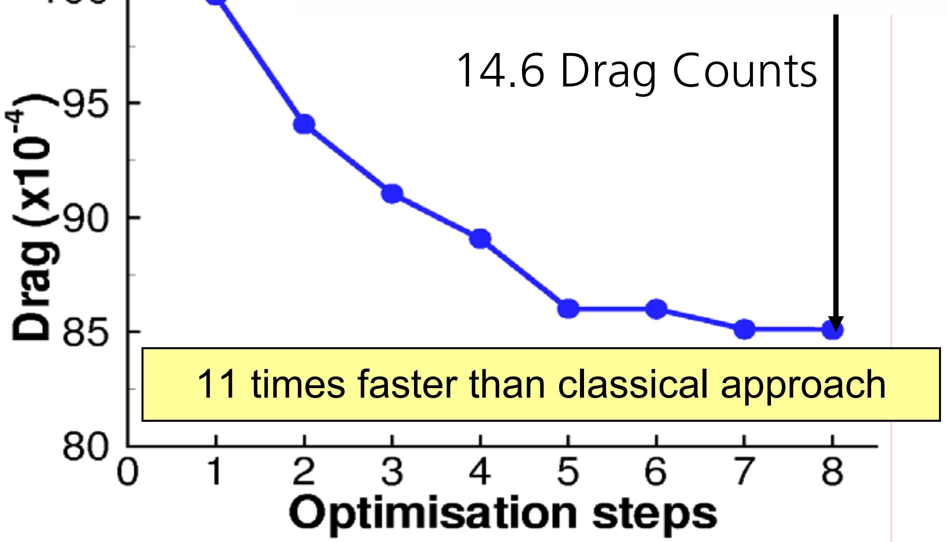
Thickness and camberline



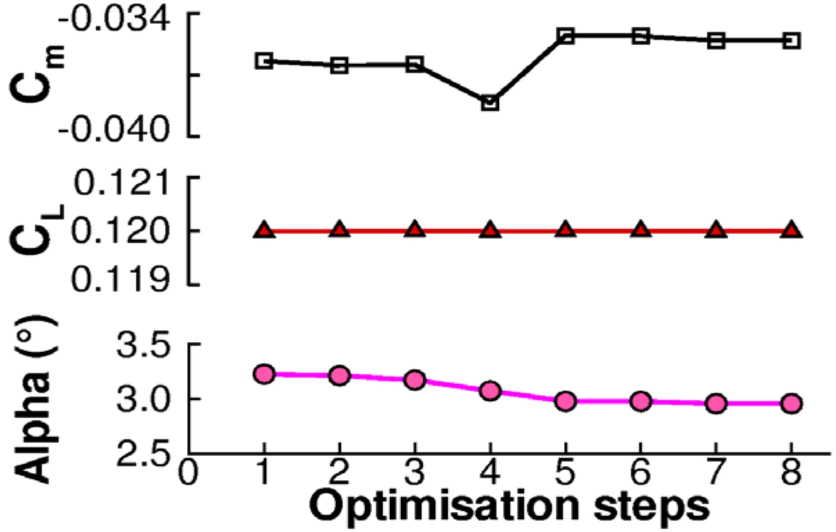
Optimization of SCT Configuration



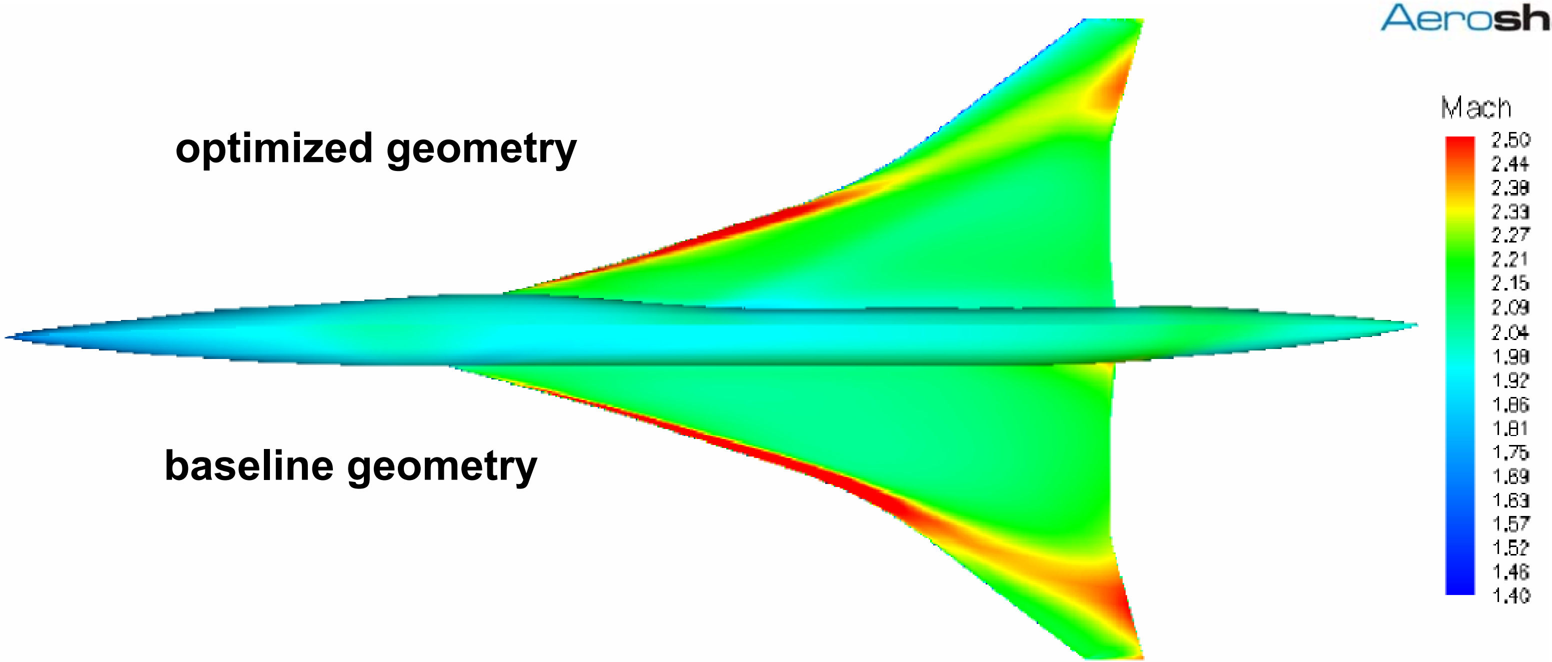


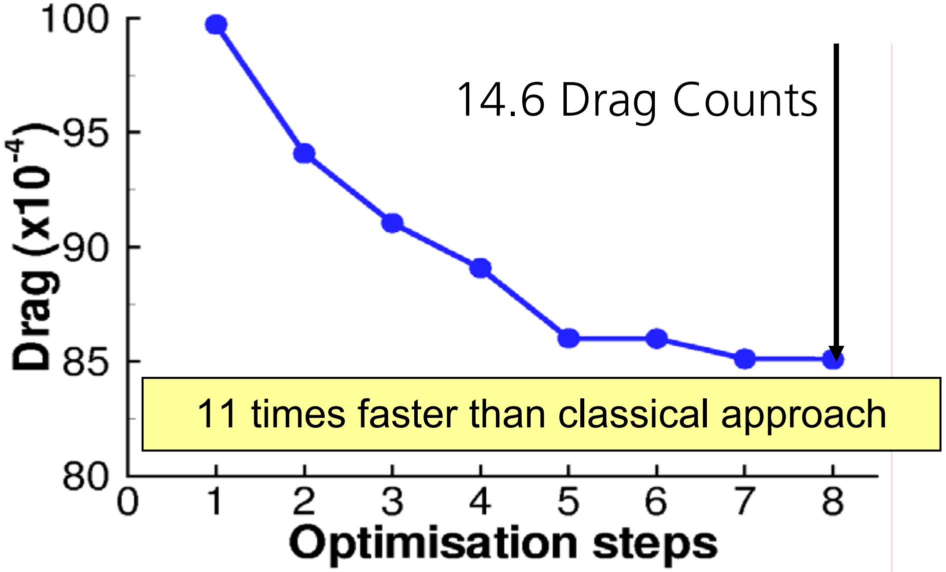
14.6 Drag Counts

11 times faster than classical approach



Optimization of SCT Configuration





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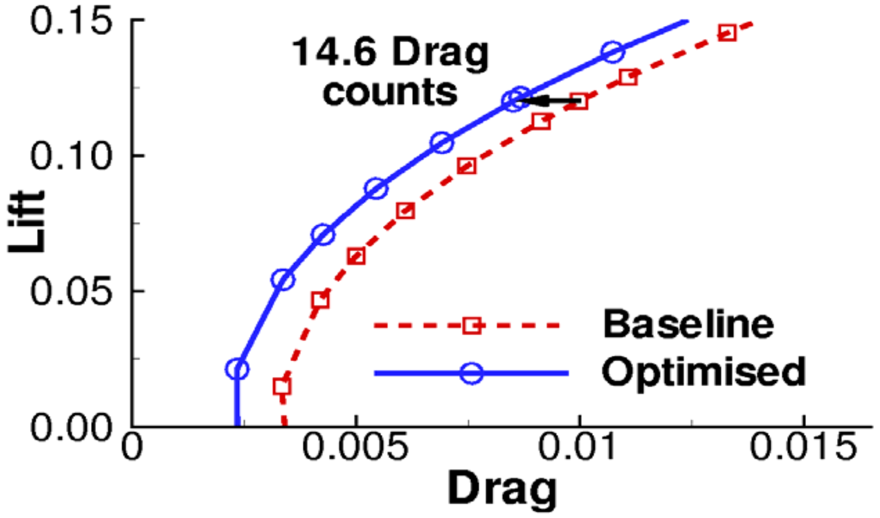
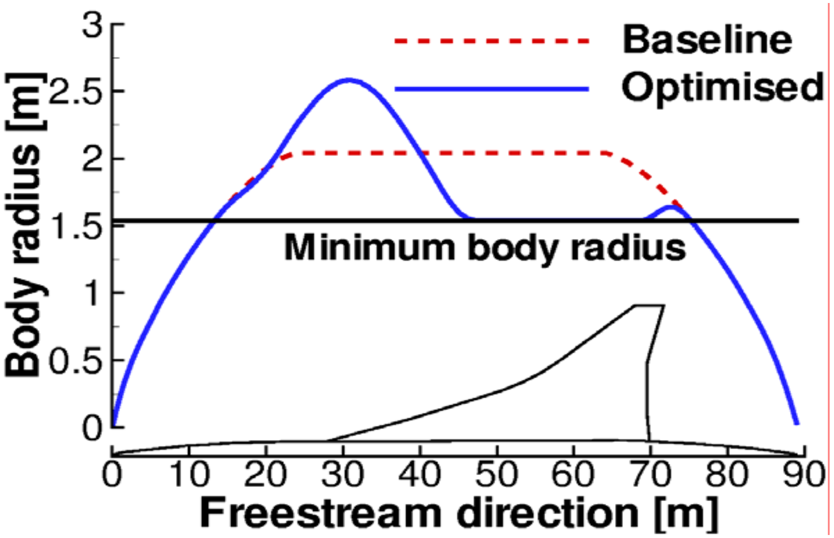
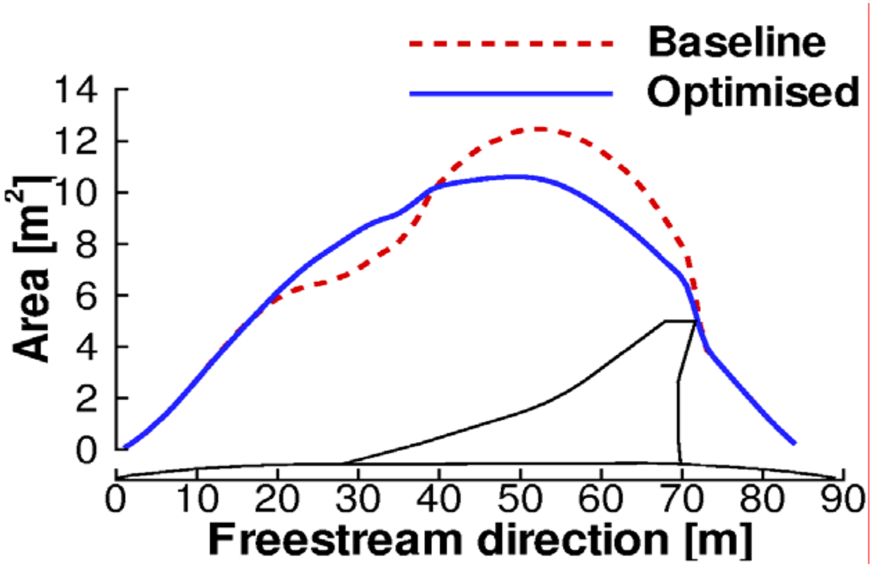


Optimization of SCT Configuration

Radius of the fuselage in freestream direction

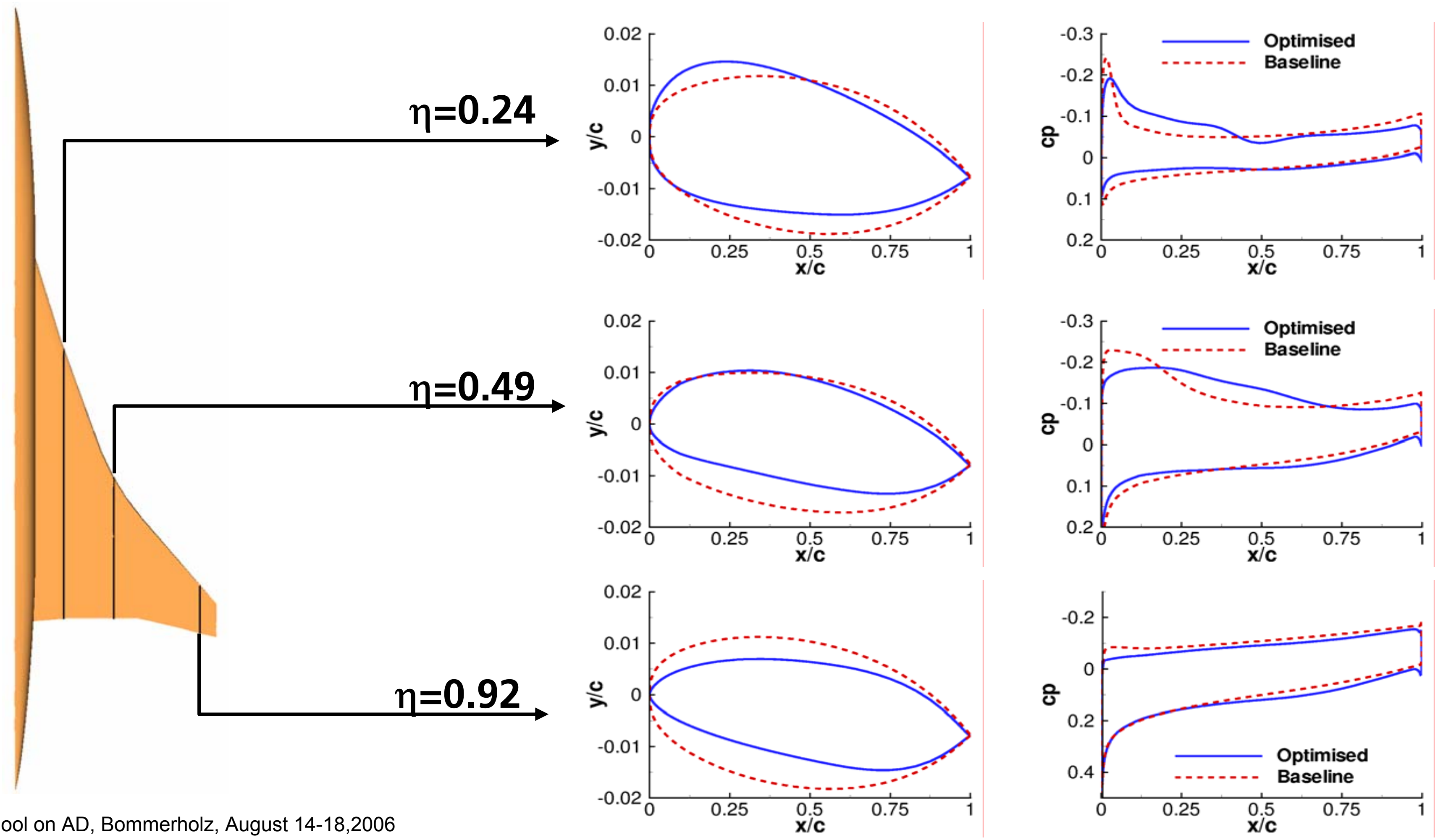
and Area Rule





Optimization of SCT Configuration

Wing section and pressure distribution



Algorithmic Differentiation (AD)

Work in progress and results

- ADFLOWer generated with TAF (3D Navier-Stokes, k-w), first verifications and validation
- Adjoint version of TAUij (2D Euler) + mesh deformation and parameterization with ADOL-C, validated and tested
- First and second derivatives of a “FLOWer-Derivate” (2D Euler) + mesh deformation and parameterization generated with TAPENADE, used for All-at-Once (Piggy-Back)
  → See lecture of Andreas Griewank!

ADFLOWer by TAF(*Fast*Opt)

Test configuration

- 2d NACA0012
- k-omega (Wilcox) turbulence model
- cell-centred metric
- 2000 time steps on fine grid
- target sensitivity: d lift/ d alpha

Steps

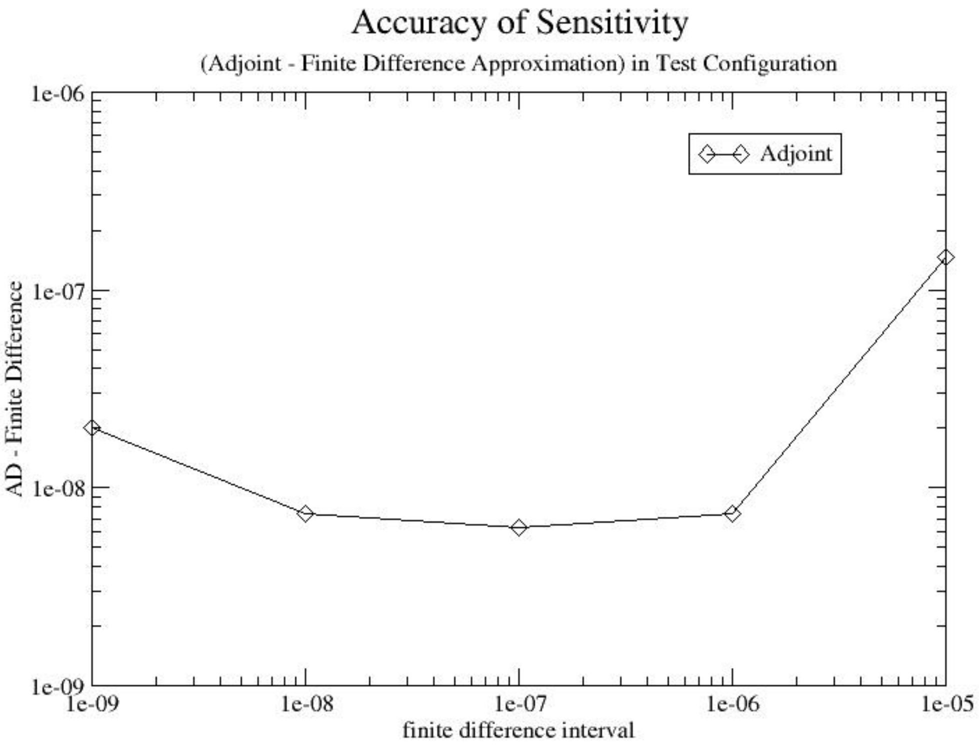
- Modifications of FLOWer code (TAF Directives, slight recoding, etc...)
- tangent-linear code (verification)
- adjoint code
- efficient adjoint code

Major challenge

- memory management (all variables in one big field 'variab') complicates detailed analysis and handling of deallocation

ADFLOWer

	TAF CPUs	Code lines	solve rel CPU	solve memory
Nominal		166000	1.0	57
tangent	293	268000	3.3	75
adjoint	253	310000	6.3	489



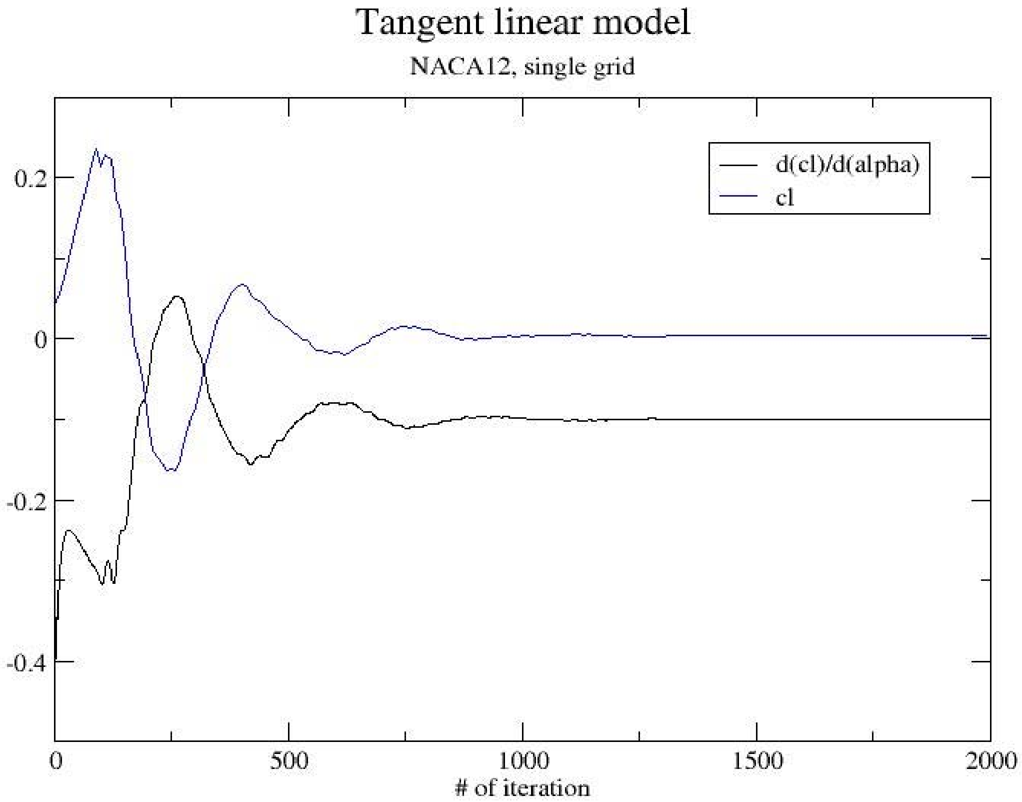
Usually better for larger configurations

Ma = 0.734
α = 2.8°
Re = 6x10^6
kw turbulence model

ADFLOWer

- Demonstrates convergence of discrete sensitivities including turbulence
- Same sensitivity for Navier-Stokes adjoint (Wilcox kw) and tangent linear model

Ma = 0.734
α = 2.8°
Re = 6x10^6
kw turbulence model



ADFLOWer

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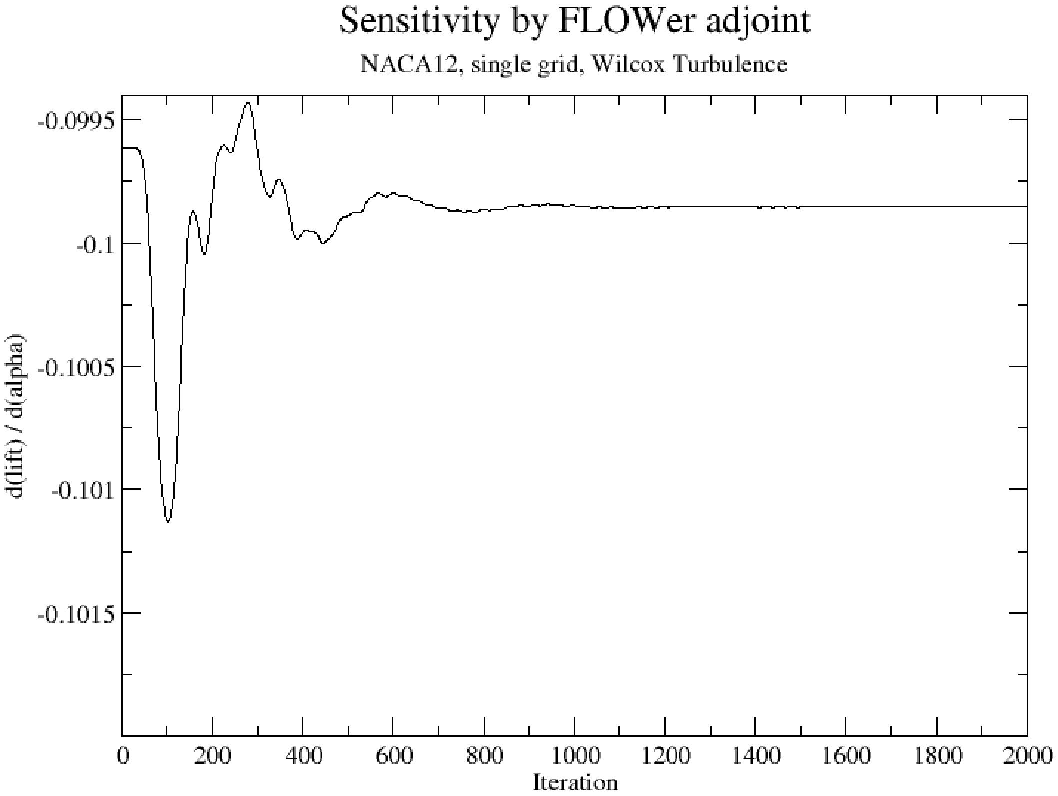


Automatic Differentiation of Entire Design Chain

$$\begin{tikzcd}
\text{design vector (P)} \arrow[r] & \text{defgeo} \arrow[r, "x_{new}"] & \text{difgeo} \arrow[r, "dx"] & \text{meshdefo} \arrow[r, "m"] & \text{flow solver} \arrow[r] & C_D \\
& \text{surface grid} \arrow[ur] & \text{grid} \arrow[ur] & & &
\end{tikzcd}$$

- **Adjoint version of entire design chain by ADOL-C (TU-Dresden)**
- **TAUij (2D Euler) + mesh deformation + parameterization**

$$\frac{dC_D}{dP} = \underset{\underset{\text{TAUij\_AD}}{\uparrow}}{\frac{\partial C_D}{\partial m}} \cdot \underset{\underset{\text{meshdefo\_AD}}{\nwarrow}}{\frac{\partial m}{\partial (dx)}} \cdot \frac{\partial (dx)}{\partial x_{new}} \cdot \underset{\underset{\text{defgeo\_AD}}{\nwarrow}}{\frac{\partial x_{new}}{\partial P}} \quad \text{and} \quad \frac{\partial (dx)}{\partial x_{new}} = \frac{\partial (x_{new} - x_{old})}{\partial x_{new}} = Id$$

Automatic Differentiation of Entire Design Chain

- Run time (2000 fixed-point iterations)
  - primal: 2 minutes
  - adjoint: 16 minutes

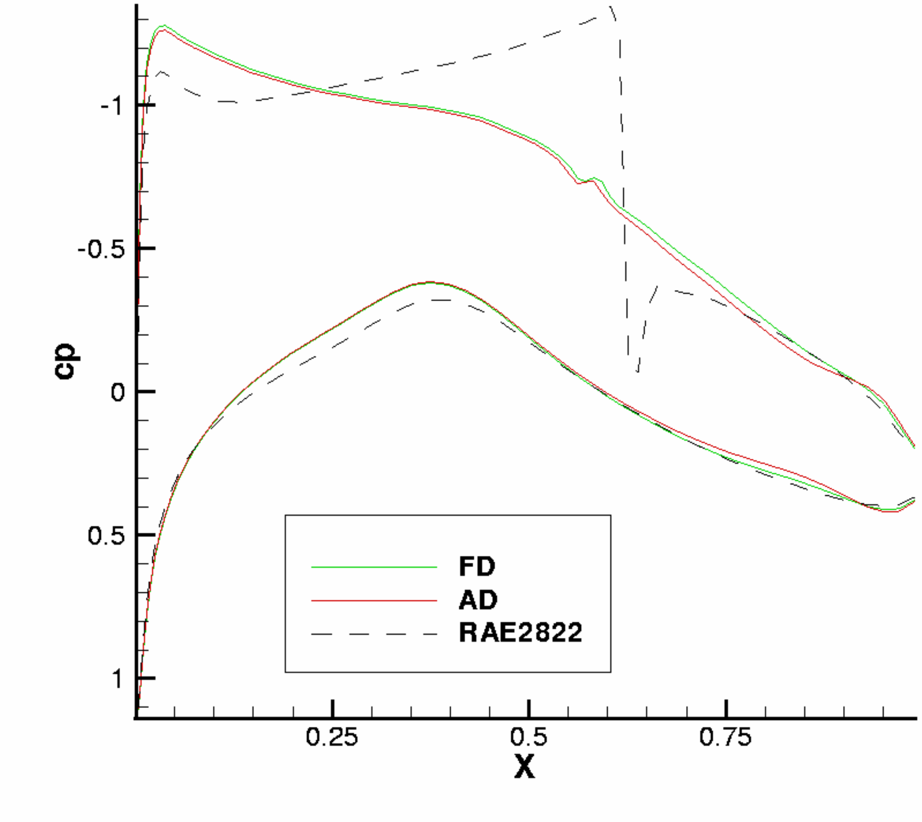
- Tape size: 340 MB (reverse accumulation approach!)

  [Christianson in 94]

- Run time memory
  - primal: 8 MB
  - adjoint: 45 MB

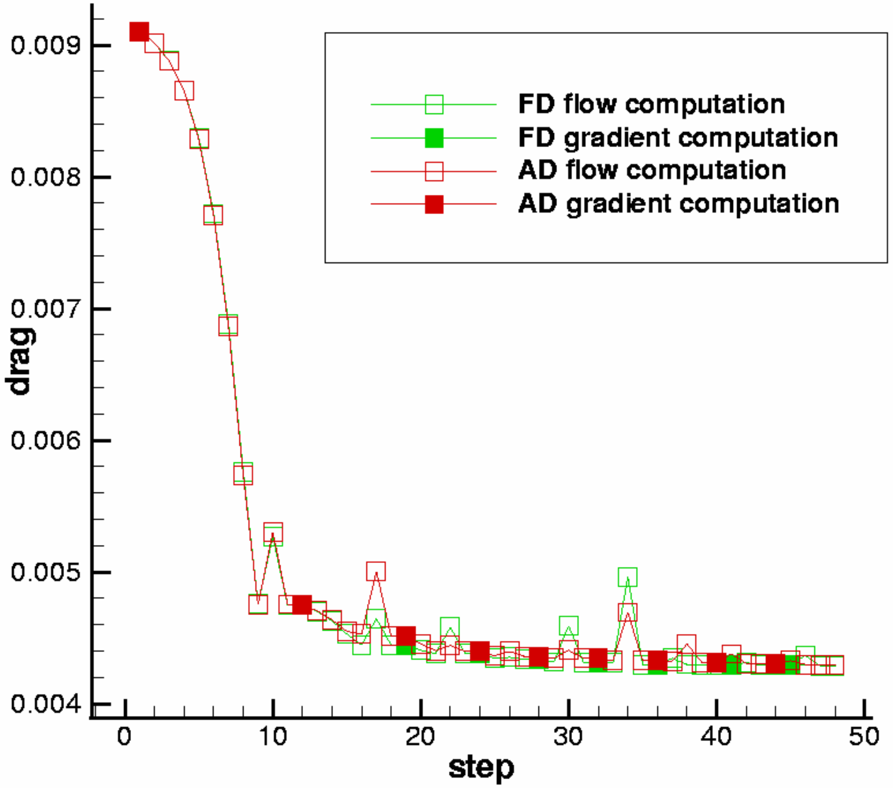
Automatic Differentiation of Entire Design Chain

First Application / Validation:



Drag reduction

- RAE 2822**,** M = 0.73, α = 2.0°
- inviscid flow, mesh 161x33 cells
- 20 design variables (Hicks-Henne)
- steepest descent



Coupled Aero-Structure Adjoint

Motivation

Wing deflection up to 7% of wing span!

Deflected aerodynamic optimal shape can be worse than the initial …

Boeing 737-800 at ground and in cruise (Ma = 0.76)

Coupled Aero-Structure Adjoint

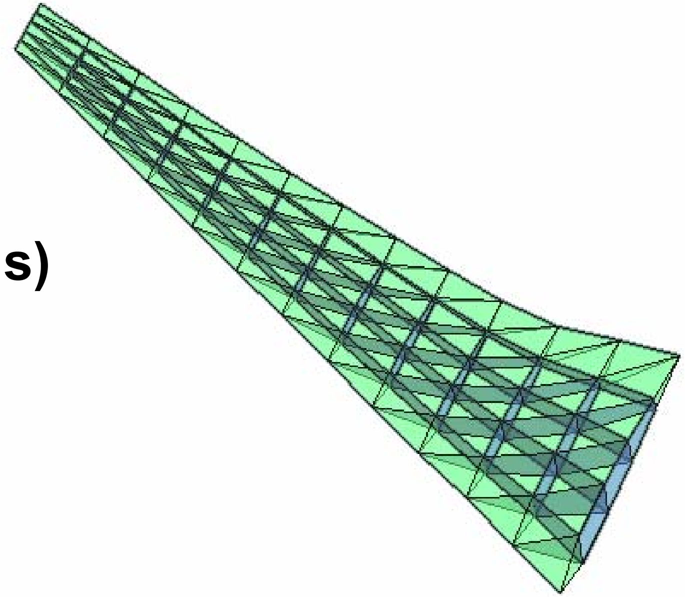
AMP wing

15 design variables (shape bumping functions based on Bernstein polynomials)

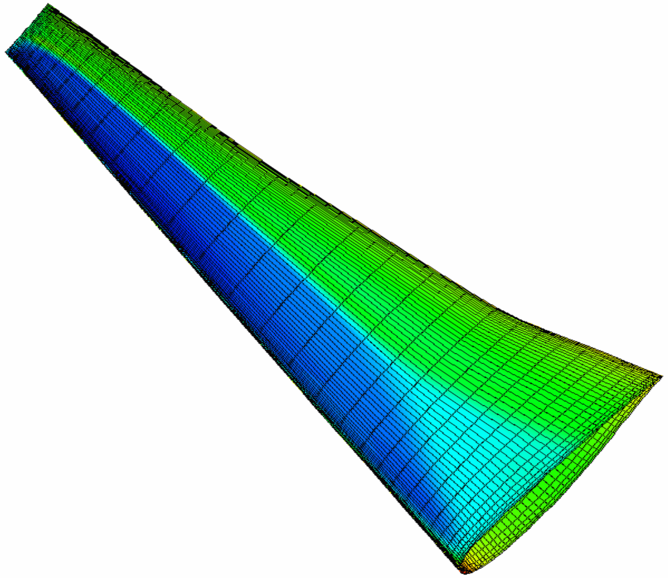
Ma=0.78
alpha=2.83

Drag reduction by constant lift

Taking into account static deformation



NASTRAN
shell/beam model
126 nodes



FLOWer MAIN/ADJOINT
15 design variables
Ma=0.78
alpha=2.83
(300.000 cells)

Coupled Aero-Structure Adjoint

Aerodynamics,
e.g Euler Eqn.: $R_A = 0$

Structure:

$$R_S = Kd - a = 0$$

K: Symmetric stiffness matrix
a: Aerodynamic force
d: Displacement vector
P: Vector of Design variables

ψ_A : **Aerodynamic Adjoint**

ψ_S : **Structure Adjoint**

~: Lagged ...

Conventional Gradient:

$$\frac{dC_D}{dP} = \frac{\partial C_D}{\partial P} + \frac{\partial C_D}{\partial w}\frac{\partial w}{\partial P} + \frac{\partial C_D}{\partial d}\frac{\partial d}{\partial P}$$

Aero/Structure Adjoint System:

$$\left(\frac{\partial R_A}{\partial w}\right)^T \psi_A = \frac{\partial C_D}{\partial w} - \left(\frac{\partial R_S}{\partial w}\right)^T \tilde{\psi}_S$$

$$\left(\frac{\partial R_S}{\partial d}\right)^T \psi_S = \frac{\partial C_D}{\partial d} - \left(\frac{\partial R_A}{\partial d}\right)^T \tilde{\psi}_A$$

Adjoint Gradient:

$$\frac{dC_D}{dP} = \frac{\partial C_D}{\partial P} - \psi_A^T \frac{\partial R_A}{\partial P} - \psi_S^T \frac{\partial R_S}{\partial P}$$

Coupled Aero-Structure Adjoint

$\frac{\partial R_A}{\partial d}, \frac{\partial R_A}{\partial P}$ **: perturb shape by d,P → calculate change in CFD residual**

$\frac{\partial C_D}{\partial d}, \frac{\partial C_D}{\partial P}$ **: perturb shape by d,P → calculate change in drag coefficient**

$\frac{\partial C_D}{\partial w}$ **: treat** $\int_C \ldots \frac{\partial p}{\partial w}(n_x \cos\alpha + n_y \sin\alpha)\ldots$ **→ boundary condition**

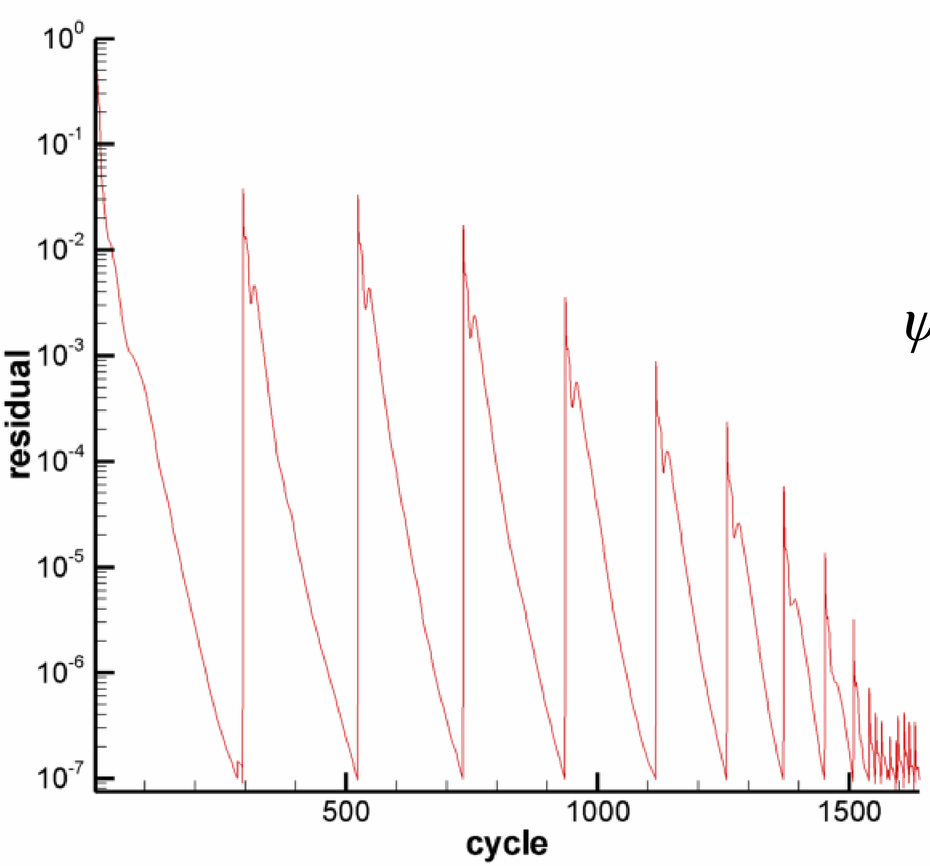
… has been derived before!

$\frac{\partial R_S}{\partial w} = \frac{\partial (Kd-a)}{\partial w} = -\frac{\partial a}{\partial w}$ **: treat** $\int_C \ldots \frac{\partial p}{\partial w} \ldots$ **→ boundary condition**

$$\frac{\partial R_S}{\partial d} = \frac{\partial (Kd-a)}{\partial d} = K = K^T$$

$$\frac{\partial R_S}{\partial P} = \frac{\partial (Kd-a)}{\partial P} = \frac{\partial K}{\partial P} d - \frac{\partial a}{\partial P}$$

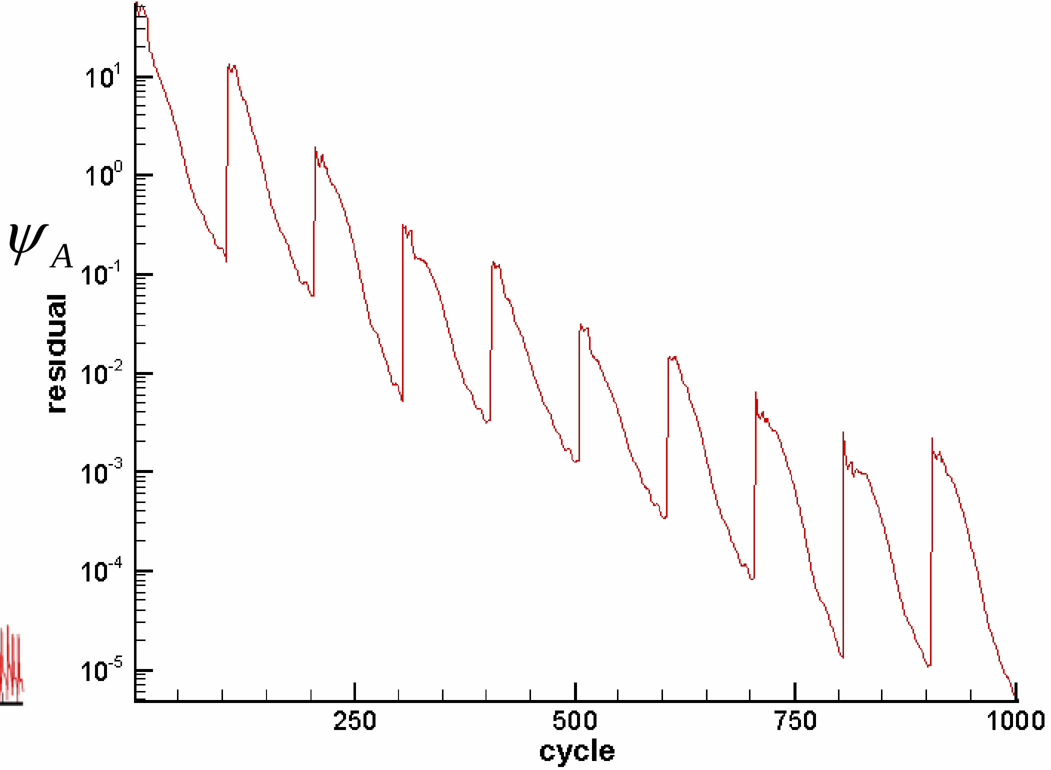
Coupled Aero-Structure Adjoint



Finite Differences:

Perturb the shape by each design variable and converge the aero-elastic loop until stationary behavior

AMP wing



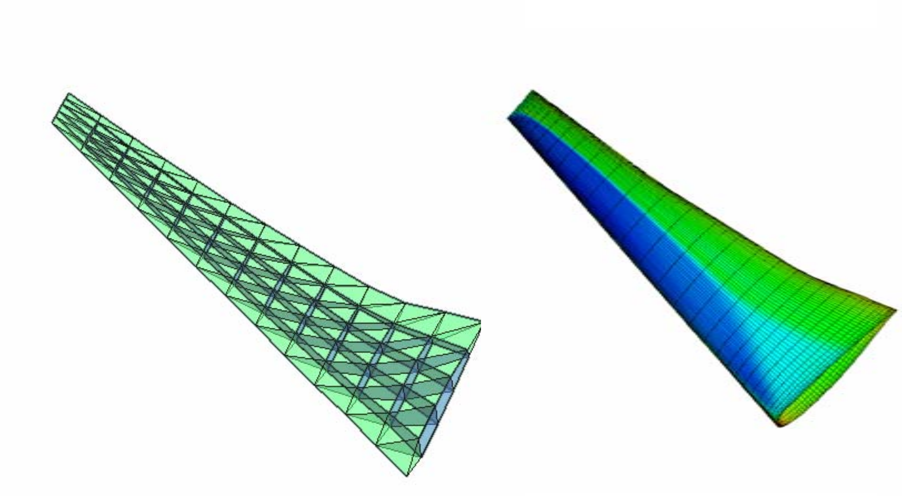
Coupled Aero-Structure Adjoint:

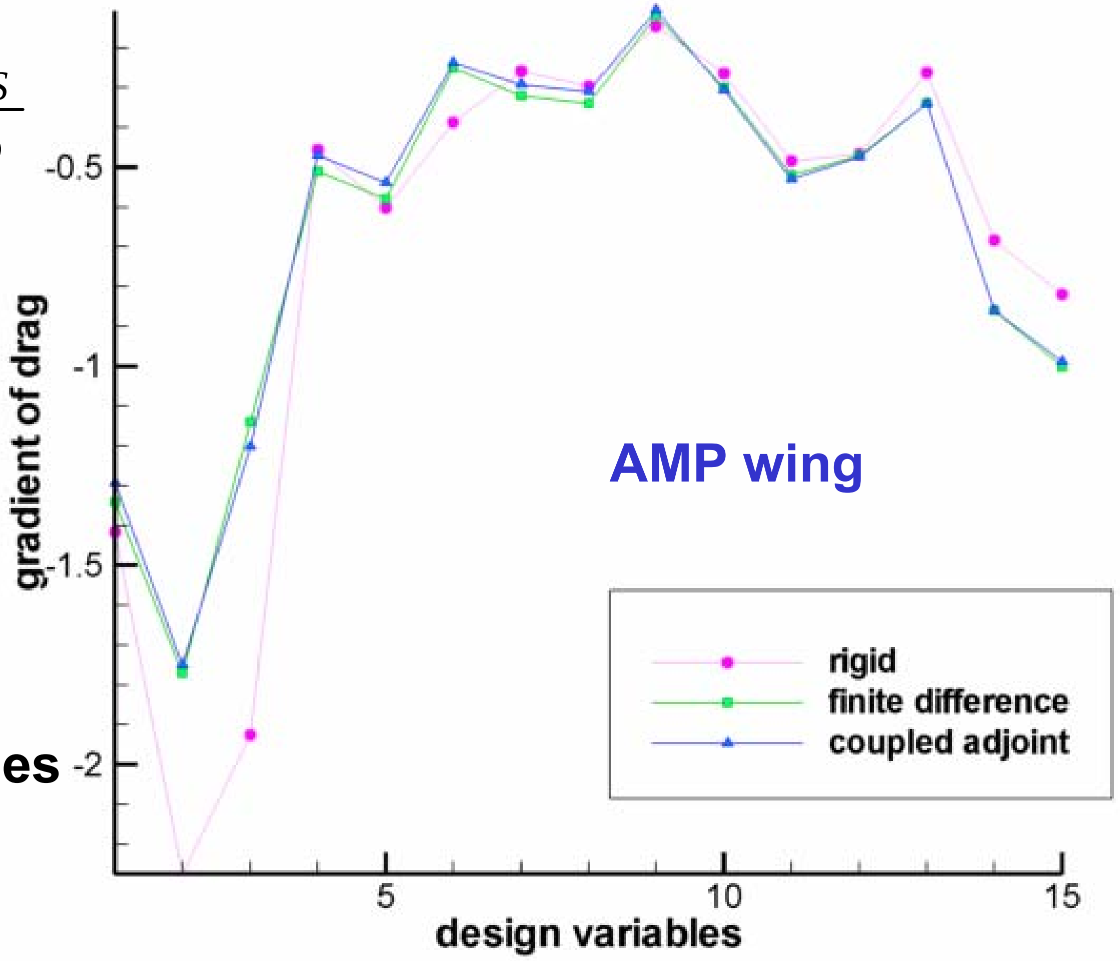
Each 100 iterations the lagged $\tilde{\psi}_S$ **is updated ...**

Coupled Aero-Structure Adjoint

Validation of Adjoint Gradient

$$\frac{dC_D}{dP} = \frac{\partial C_D}{\partial P} - \psi_A^T \frac{\partial R_A}{\partial P} - \psi_S^T \frac{\partial R_S}{\partial P}$$





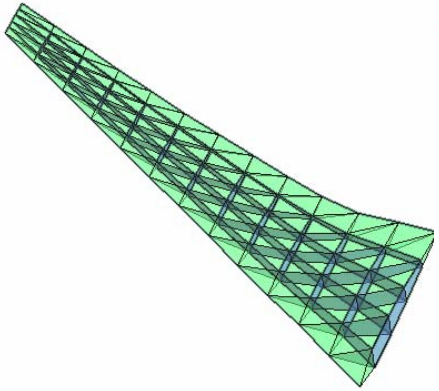
NASTRAN
shell/beam model
126 nodes

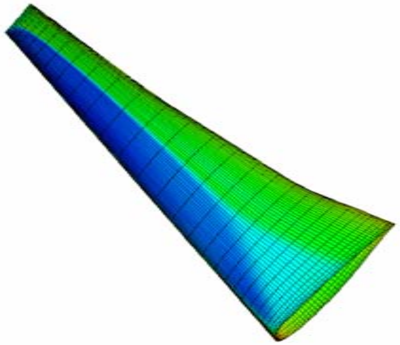
15 design variables
Ma=0.78
alpha=2.83
(300.000 cells)

Coupled Aero-Structure Adjoint

Validation of Adjoint Gradient

$$\frac{dC_L}{dP} = \frac{\partial C_L}{\partial P} - \psi_A^T \frac{\partial R_A}{\partial P} - \psi_S^T \frac{\partial R_S}{\partial P}$$





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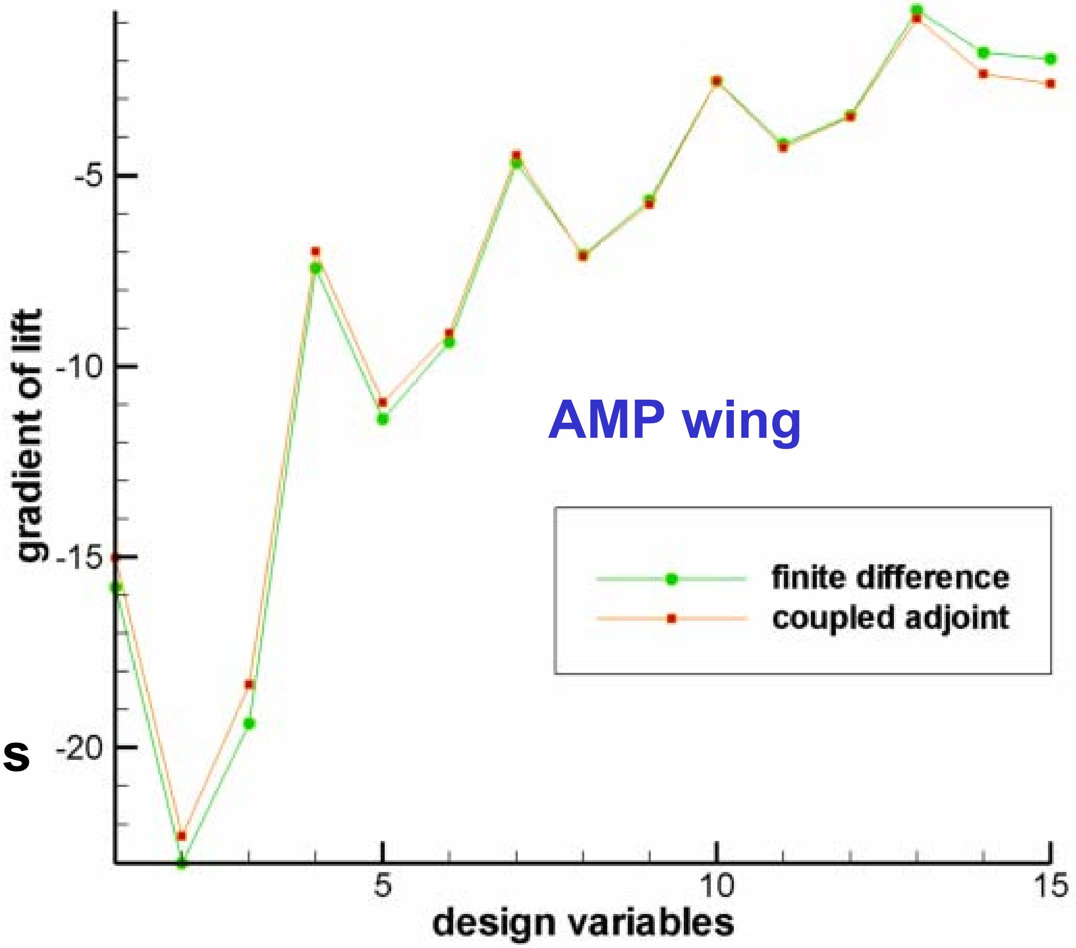


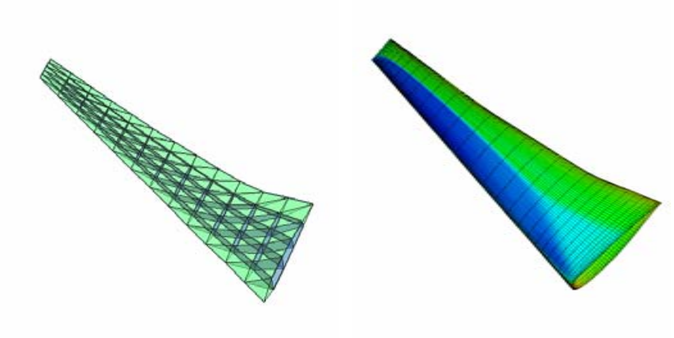
Coupled Aero-Structure Adjoint

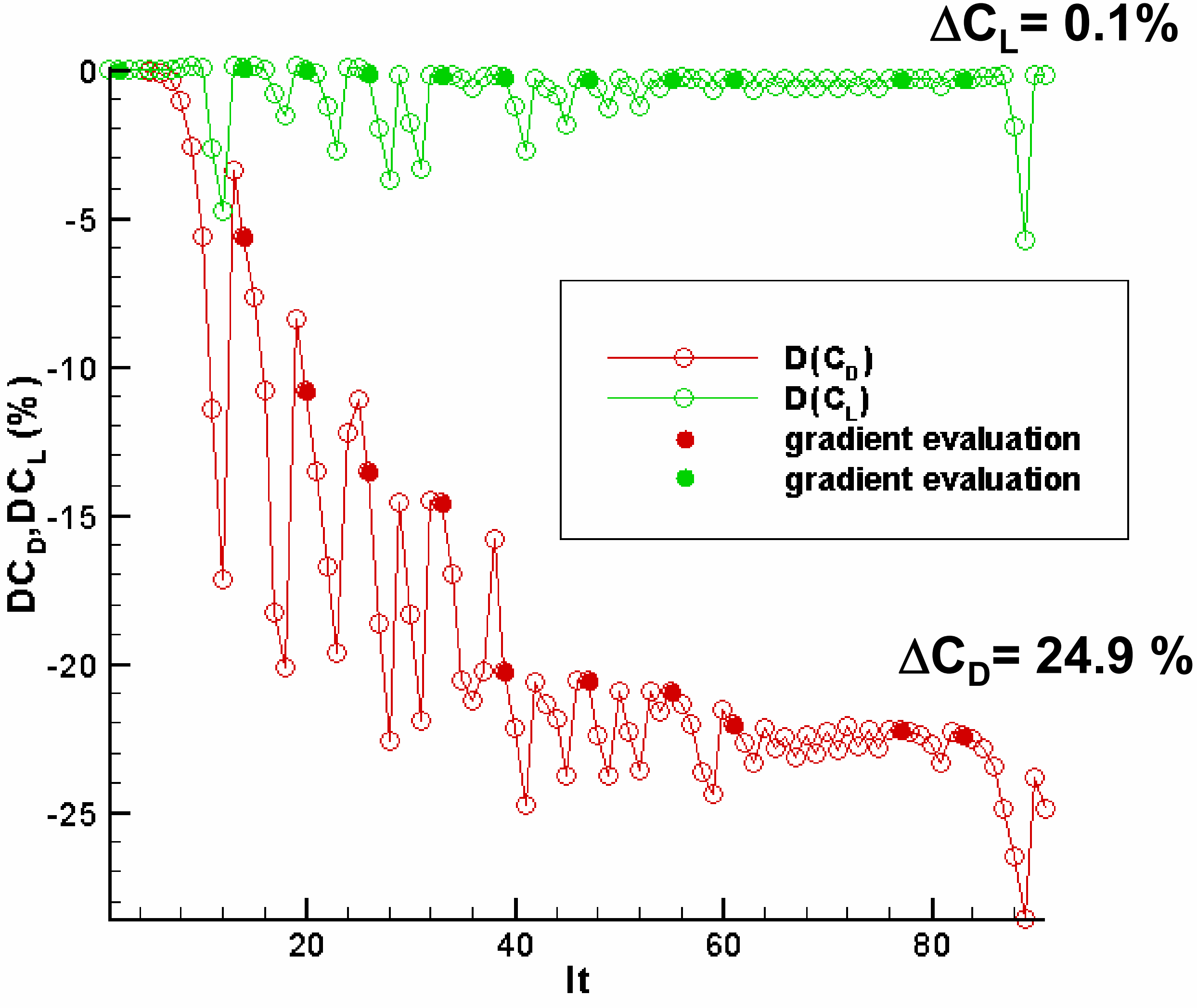
AMP wing

240 design variables (control points free form deformation)

Ma=0.78
alpha=2.83

Drag reduction by constant lift





feasible direction method

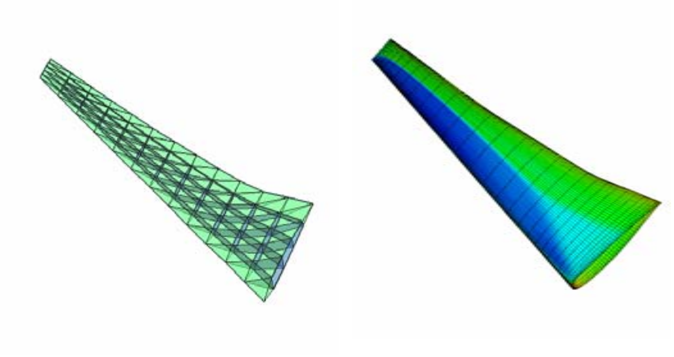
Coupled Aero-Structure Adjoint

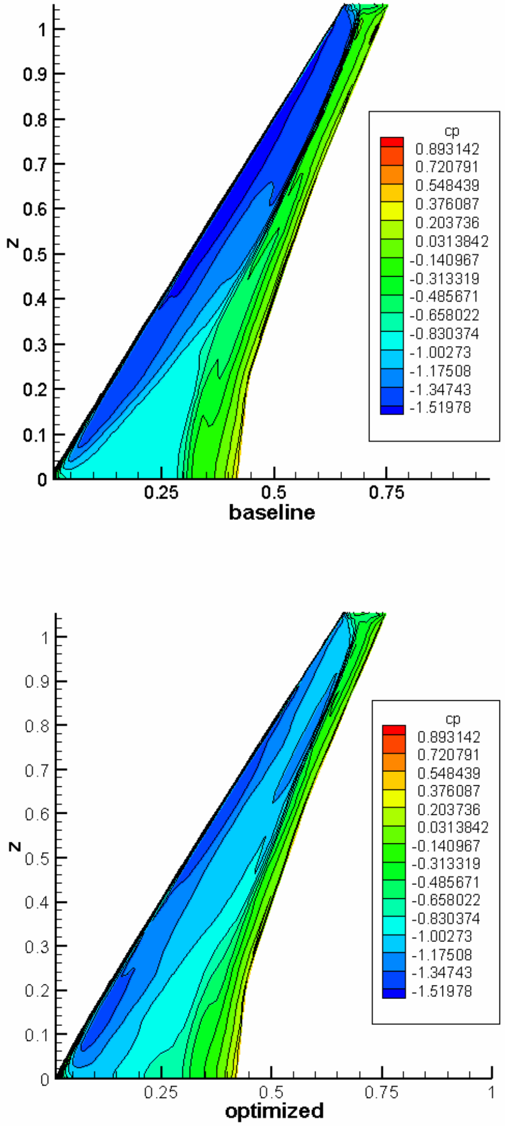
AMP wing

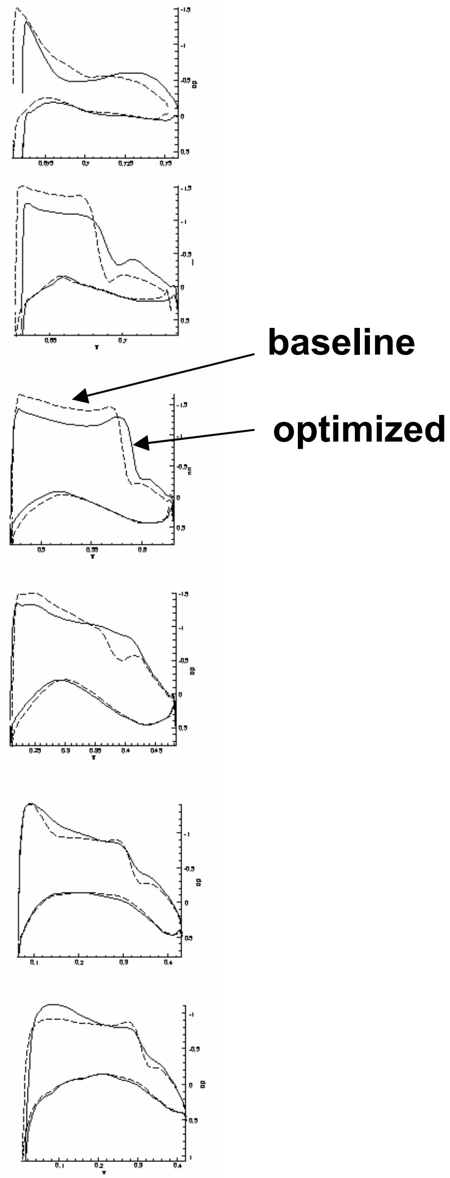
240 design variables (control points free form deformation)

Ma=0.78
alpha=2.83

Drag reduction by constant lift







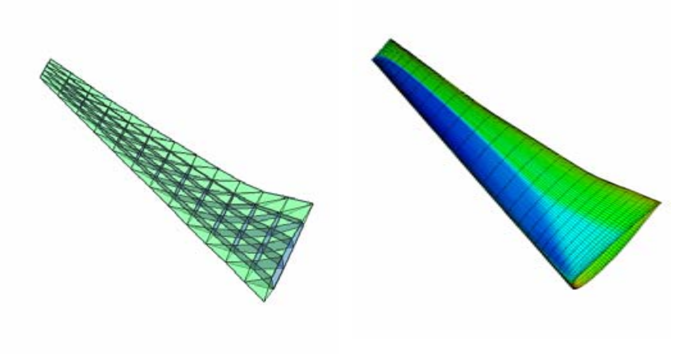
Coupled Aero-Structure Adjoint

AMP wing

240 design variables
(control points free form
deformation)

Ma=0.78
alpha=2.83

Drag reduction by
constant lift



Comparison of numerical effort:
(PC Pentium IV, 2.6 GHz, 2GB RAM)

- **Coupled adjoint: 15 days**
  (11 gradient and 91 state evaluations)
- **Finite differences: 227 days**

Aero-Structure MDO

Range R:

$$R \propto \frac{C_L}{C_D} \ln \frac{W}{W-F} = \frac{C_L}{C_D} \ln \left(\frac{1+\lambda\, ks}{1+\lambda\, ks - \frac{F}{W_0}} \right)$$

Fuel Weight F

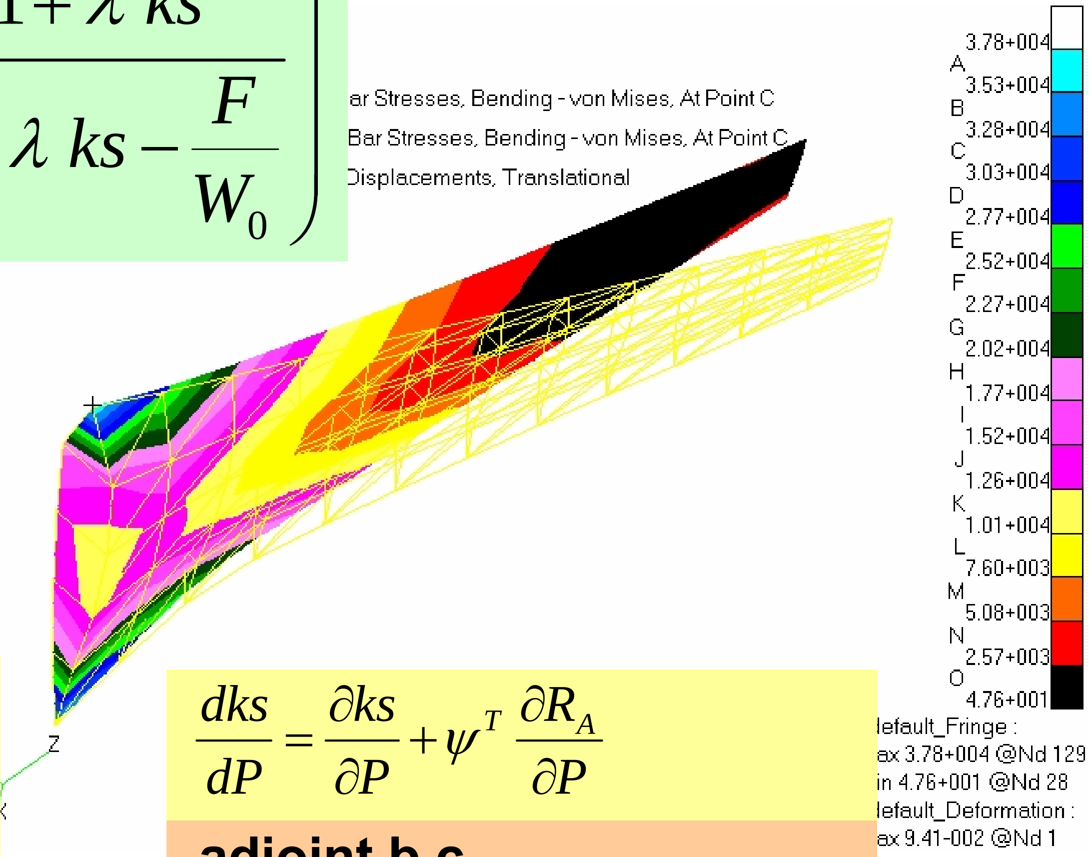
Weight W:

$$W = W_0 (1+\lambda\, ks)$$

Kreisselmeier-Steinhauser:

$$ks = \frac{1}{\beta} \ln\Big(\sum_n \exp\Big(\beta \frac{\sigma_n - \sigma_0}{\sigma_0}\Big)\Big)$$

λ=0.2 , σ_0 =30.000 and β=40



$$\frac{dks}{dP} = \frac{\partial ks}{\partial P} + \psi^T \frac{\partial R_A}{\partial P}$$

adjoint b.c.

$$n_x \psi_2 + n_y \psi_3 + n_z \psi_4 = -\frac{\partial ks}{\partial p}$$

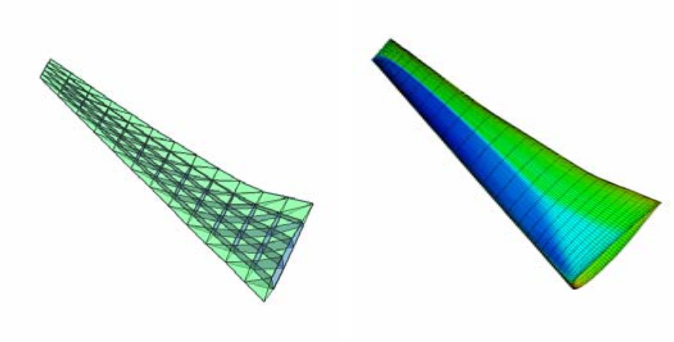
Aero-Structure MDO

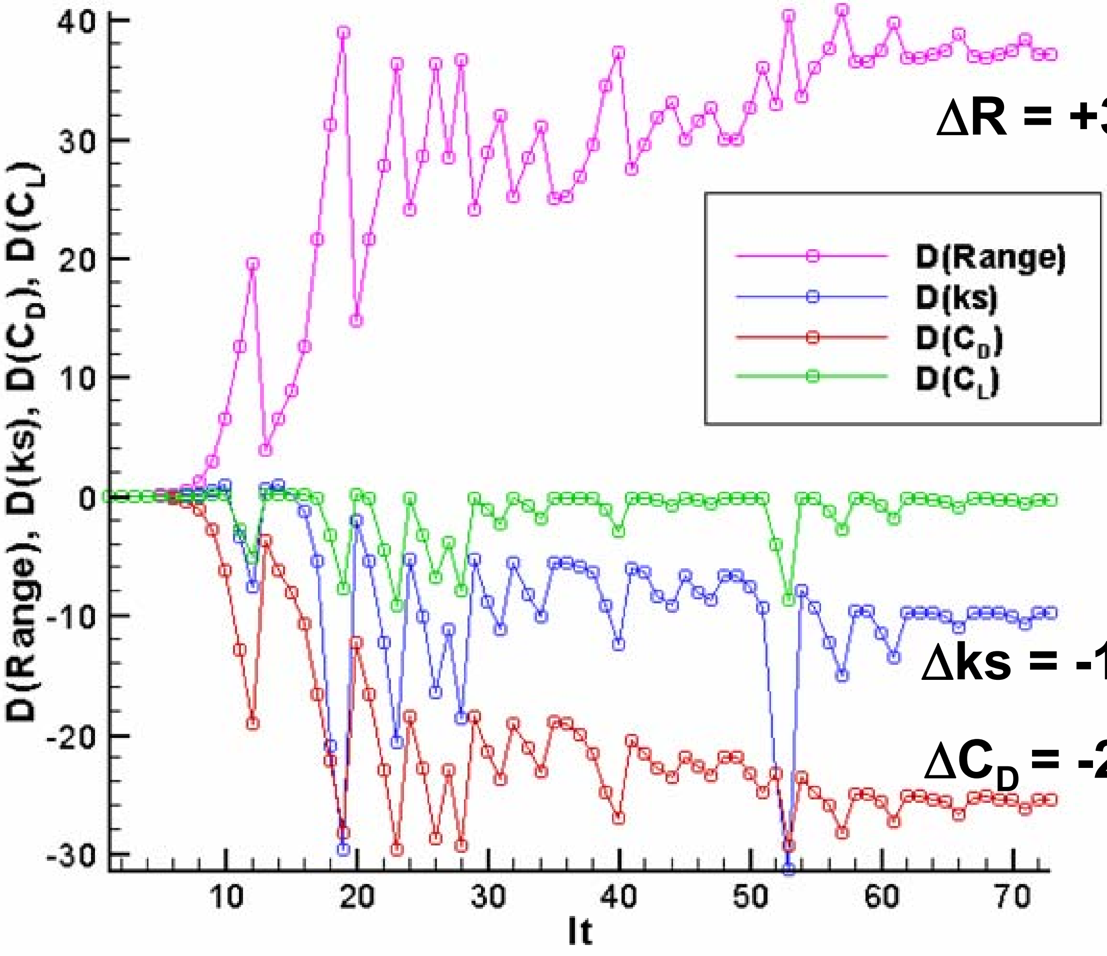
AMP wing

240 design variables (control points free form deformation)

Ma=0.78
alpha=2.83

Range maximization by constant lift





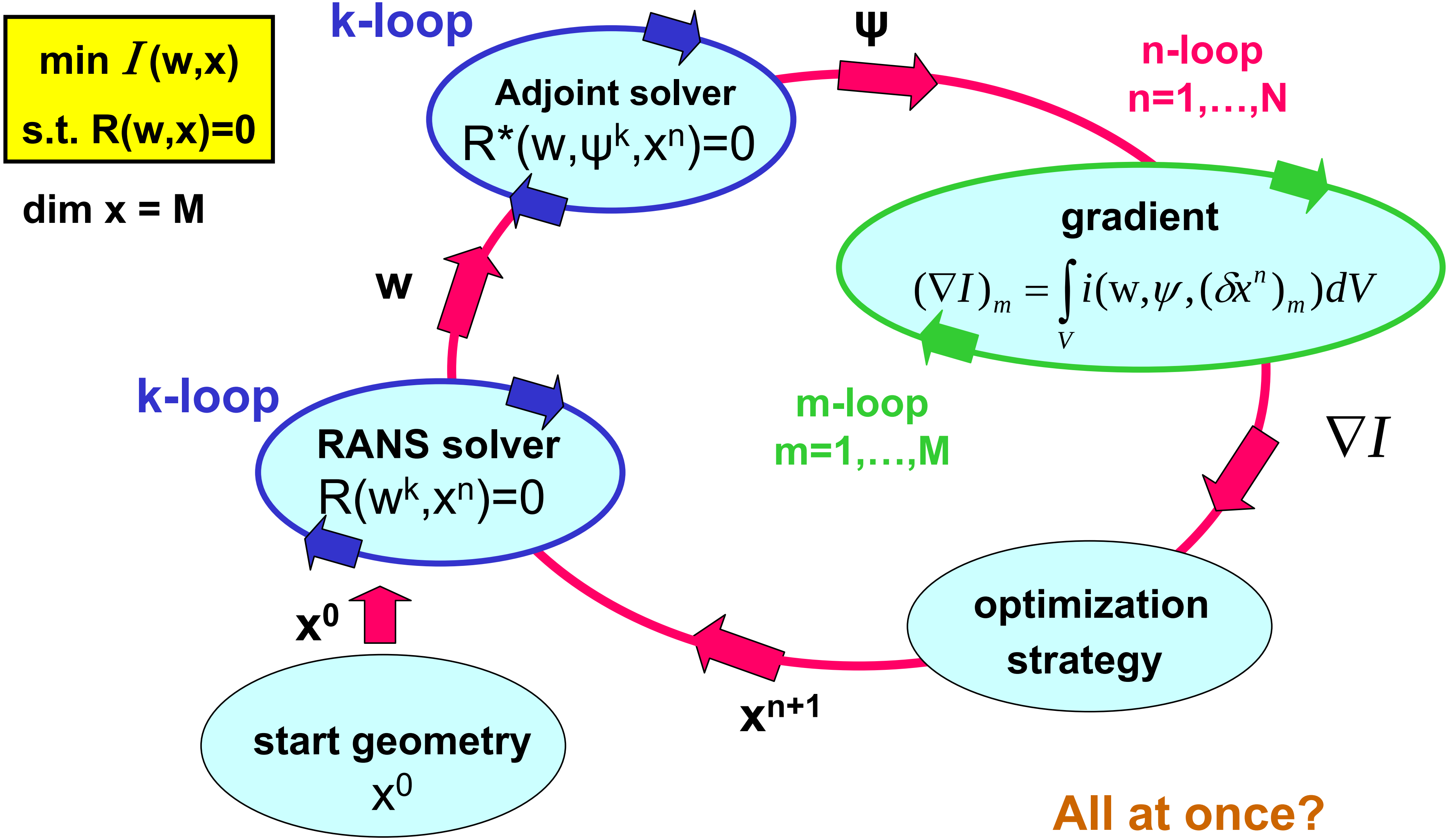
ΔR = +37 %

Δks = -10 %

ΔC_D = -25 %

feasible direction method

Adjoint Based Optimization



All at once?

Simultaneous Pseudo-Time stepping
- One Shot Approach -

min I(w,x)

s.t. R(w,x)=0

dim x = M

$$L(w,x,\psi) = I(w,x) - \psi^T R(w,x)$$

KKT

$\nabla_w L(w,x,\psi) = 0$ **(adjoint equation)**

$\nabla_x L(w,x,\psi) = 0$ **(design equation)**

$R(w,x) = 0$ **(state equation)**

$$\begin{bmatrix} w+\Delta w \\ x+\Delta x \\ \psi+\Delta\psi \end{bmatrix} = \begin{bmatrix} w \\ x \\ \psi \end{bmatrix} - \begin{bmatrix} L_{ww} & L_{wx} & (\partial R/\partial w)^T \\ L_{xw} & L_{xx} & (\partial R/\partial x)^T \\ \partial R/\partial w & \partial R/\partial x & 0 \end{bmatrix}^{-1} \begin{bmatrix} \nabla_w L \\ \nabla_x L \\ R \end{bmatrix}$$

Newton SQP method

$$\begin{bmatrix} \Delta w \\ \Delta x \\ \Delta\psi \end{bmatrix} = \begin{bmatrix} 0 & 0 & I \\ 0 & B & (\partial R/\partial x)^T \\ I & \partial R/\partial x & 0 \end{bmatrix}^{-1} \begin{bmatrix} -\nabla_w L \\ -\nabla_x L \\ -R \end{bmatrix}$$

inexact Newton rSQP method

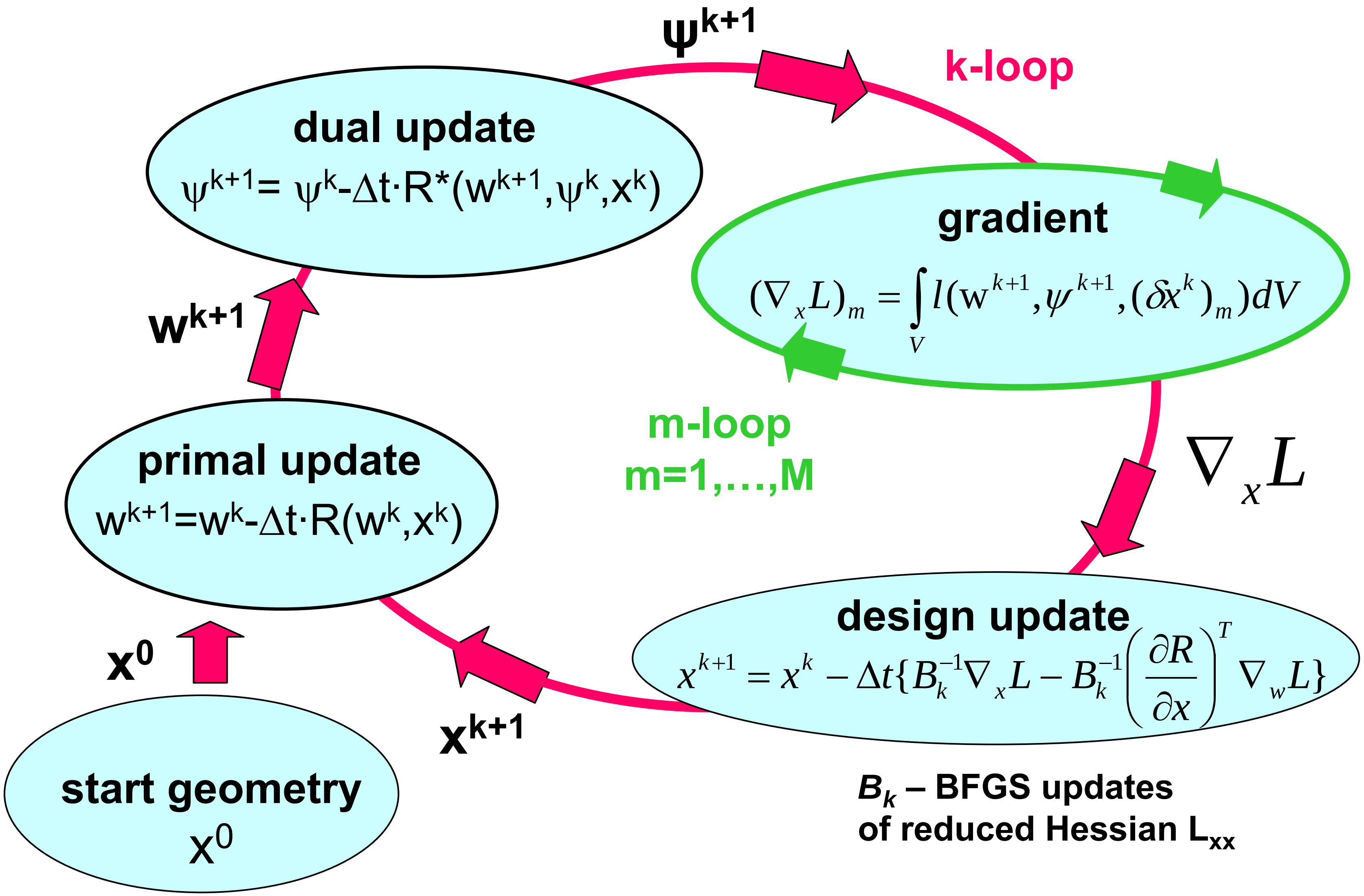
⇕

simultaneous preconditioned pseudo time stepping

DLR

Simultaneous Pseudo-Time stepping
- One Shot Approach -

University of Trier



ψ^{k+1}

k-loop

dual update

$\psi^{k+1} = \psi^k - \Delta t \cdot R^*(w^{k+1}, \psi^k, x^k)$

gradient

$$(\nabla_x L)_m = \int_V l(w^{k+1}, \psi^{k+1}, (\delta x^k)_m)\, dV$$

w^{k+1}

m-loop
m=1,…,M

$\nabla_x L$

primal update

$w^{k+1} = w^k - \Delta t \cdot R(w^k, x^k)$

design update

$$x^{k+1} = x^k - \Delta t\{B_k^{-1} \nabla_x L - B_k^{-1} \left(\frac{\partial R}{\partial x} \right)^T \nabla_w L\}$$

x^0

x^{k+1}

start geometry

x^0

B_k – BFGS updates
of reduced Hessian L_{xx}

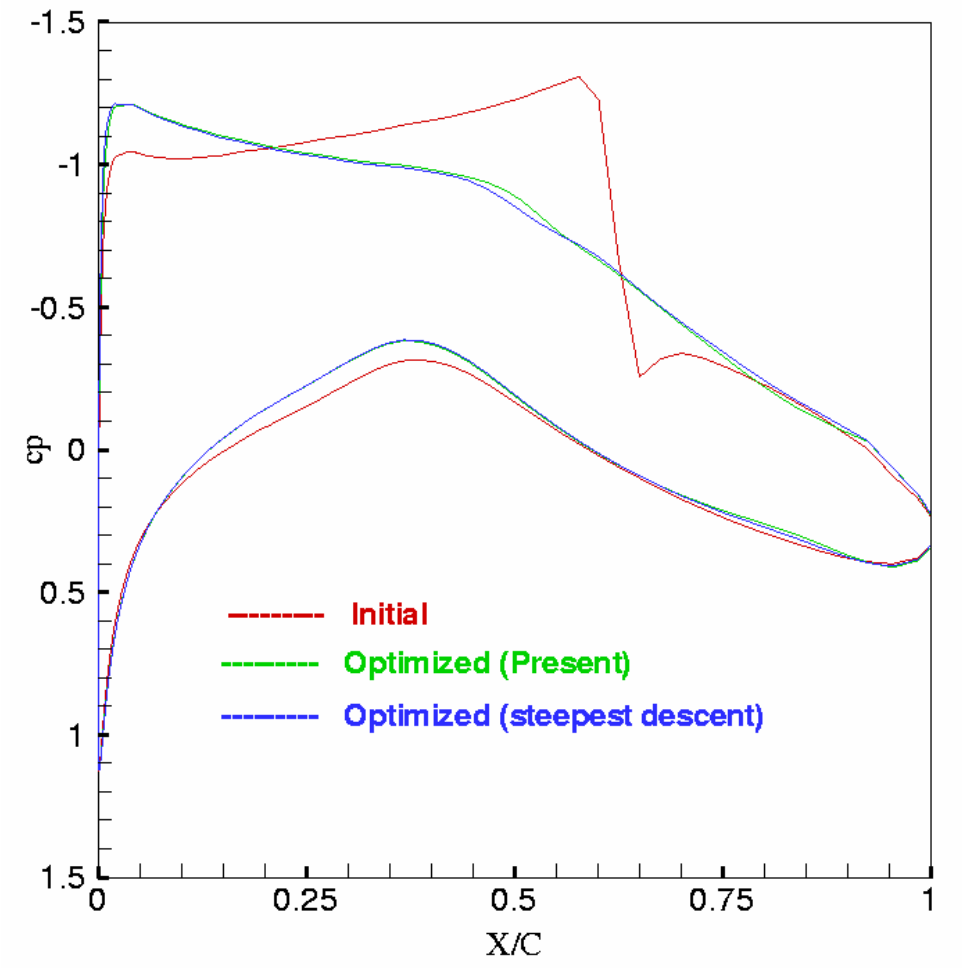
Simultaneous Pseudo-Time stepping
- One Shot Approach -

Optimization problem

- **drag reduction for RAE 2822**
- **inviscid flow**
- **M=0.73, a=2^0**

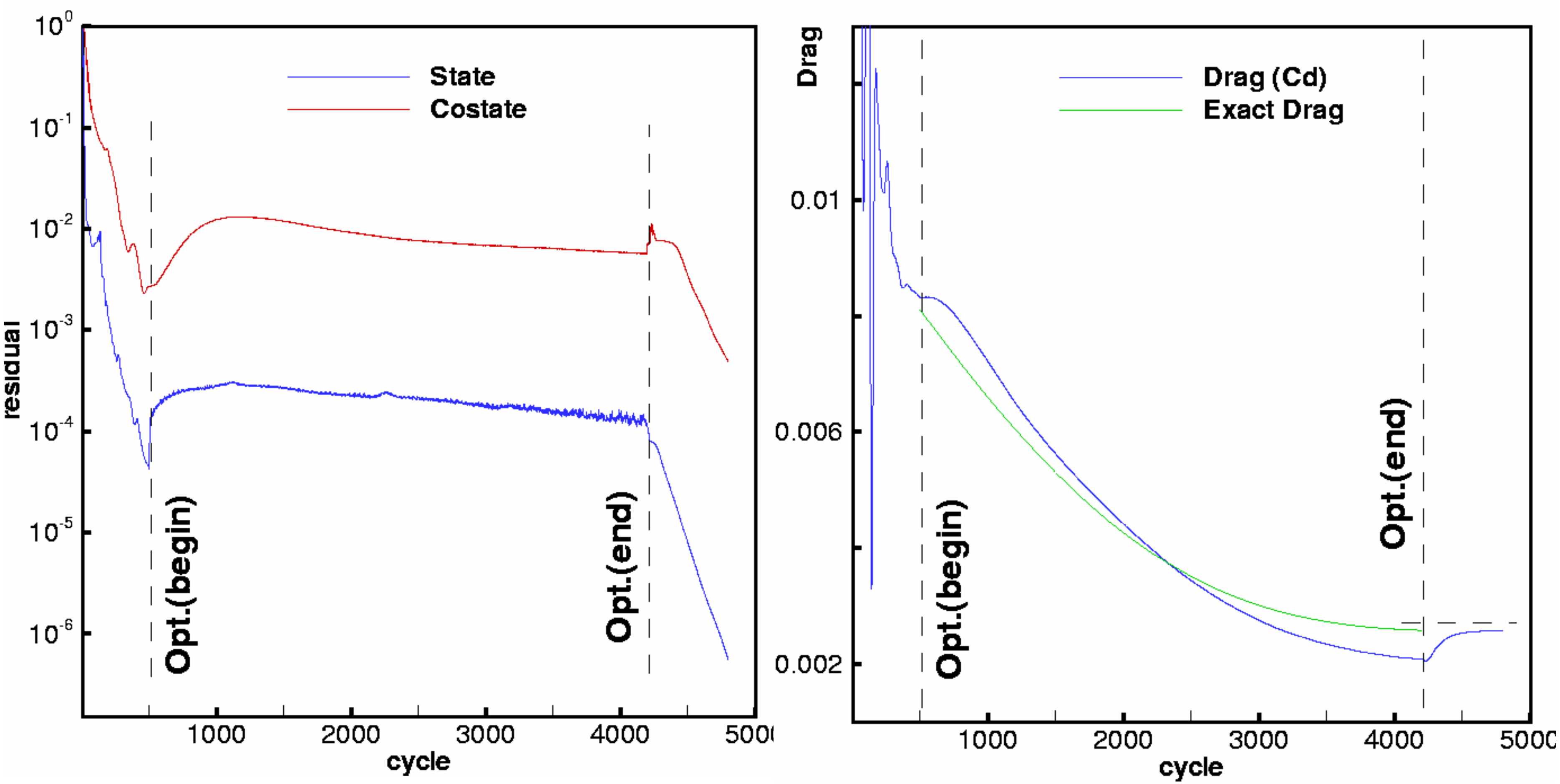
Tools

- **FLOWer**
- **FLOWer adjoint**



Simultaneous Pseudo-Time stepping
- One Shot Approach -

University of Trier



Optimization at the cost of 4 flow simulations!