Constrained Single-Step One-Shot Method with Applications in Aerodynamics

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Collaborators

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Problem Statement

Goal: $\min_u f(y,u)$ **s.t.** $c(y,u)=0,$

where y and u are the state and design variables.

Given fixed point iteration $y_{k+1}=G(y_k,u)$ (e.g. pseudo-time stepping) to solve PDE $c(y,u)=0.$

Assumptions:

- $\frac{\partial c}{\partial y}$ **always invertible. IFT $\Rightarrow$ given $u, \exists! \, y$ s.t.** $c(y,u)=0.$
- $G, f \in C^{2,1}.$
- G **contractive:** $\|G_y(y,u)\| = \|G_y^T(y,u)\| \le \rho < 1$

One-Shot approach

$$L(y,\bar{y},u) = f(y,u) + (G(y,u) - y)^T \bar{y}$$
$$= \underbrace{N(y,\bar{y},u)}_{\text{shifted Lagragian}} - y^T \bar{y}$$

Stationary point:
$$\begin{cases} L_{\bar{y}} = G(y,u) - y = 0 \\ L_y = N_y(y,\bar{y},u)^T - \bar{y} = 0 \\ L_u = N_u(y,\bar{y},u)^T = 0 \end{cases}$$

One-step one-shot (step *k+1*):

$$(OS)\begin{cases} y_{k+1} = G(y_k, u_k) & \text{primal update} \\ \bar{y}_{k+1} = N_y(y_k, \bar{y}_k, u_k)^T & \text{dual update} \\ u_{k+1} = u_k - B_k^{-1} N_u(y_k, \bar{y}_k, u_k)^T & \text{design update} \end{cases}$$

Aims: **Choose *B* such that:**
- **Convergence of *(OS)*.**
- **Bounded retardation.**

Bounded retardation

Jacobian of the extended iteration:

$$J_* = \left. \frac{\partial(y_{k+1}, \bar{y}_{k+1}, u_{k+1})}{\partial(y_k, \bar{y}_k, u_k)} \right|_{(y^*, \bar{y}^*, u^*)} = \begin{pmatrix} G_y & 0 & G_u \\ N_{yy} & G_y^T & N_{yu} \\ -B^{-1}N_{uy} & -B^{-1}G_u^T & I - B^{-1}N_{uu} \end{pmatrix}$$

Whenever we can define B **such that**

$$\frac{1-\rho(G_y)}{1-\hat{\rho}(J_*)} < const$$

we have bounded retardation.

Necessary condition for contractivity

Eigenvalues of J_* are the zeros of the equation

$$\det((\lambda - 1)B + H(\lambda)) = 0$$

where

$$H(\lambda) = \left(-G_u^T (G_y^T - \lambda I)^{-1}, I\right) \begin{pmatrix} N_{yy} & N_{yu} \\ N_{uy} & N_{uu} \end{pmatrix} \begin{pmatrix} -(G_y - \lambda I)^{-1} G_u \\ I \end{pmatrix}.$$

Necessary (but not sufficient) condition for contractivity:

$$B = B^T \succ 0 \qquad \textbf{and} \qquad B \succ \frac{1}{2} H(-1).$$

[Griewank, 2006]

Exact penalty function: L^a

Remark:

Deriving (sufficient) conditions on B for J_* to have a spectral radius smaller than 1 has proven difficult.

Instead, we look for descent on the augmented Lagrangian

$$L^a(y,\bar{y},u) := \frac{\alpha}{2}\underbrace{\left\|G(y,u)-y\right\|^2}_{\text{primal residual}} + \frac{\beta}{2}\underbrace{\left\|N_y(y,\bar{y},u)^T-\bar{y}\right\|^2}_{\text{dual residual}} + \underbrace{N-\bar{y}^T y}_{\text{Lagrangian}},$$

where $\alpha > 0$ and $\beta > 0$.

Correspondence condition

The full gradient of L^a is given by

$$\begin{bmatrix} \nabla_y L^a \\ \nabla_{\bar{y}} L^a \\ \nabla_u L^a \end{bmatrix} = -Ms(y,\bar{y},u), \quad \textbf{where} \quad s(y,\bar{y},u) = \begin{bmatrix} G(y,u) - y \\ N_y(y,\bar{y},u)^T - \bar{y} \\ -B^{-1} N_u(y,\bar{y},u)^T \end{bmatrix}$$

and $$M = \begin{bmatrix} \alpha(I - G_y{}^T), & -I - \beta N_{yy}, & 0 \\ -I, & \beta(I - G_y), & 0 \\ -\alpha G_u{}^T, & -\beta N_{yu}{}^T & B \end{bmatrix}.$$

Correspondence condition

Consequence (Correspondence condition):

There is a 1-1 correspondence between the stationary points of L^a and the roots of s if

$$\det[\alpha\beta(I - G_y{}^T)(I - G_y) - I - \beta N_{yy}] \neq 0,$$

for which it is sufficient that

$$\alpha\beta(1-\rho)^2 > 1 + \beta \left\| N_{yy} \right\|.$$

[Hamdi, Griewank, 2008]

Descent condition

Theorem (Descent condition):

$s(y,\bar{y},u)$ **is a descent direction for all large positive** B

if and only if

$$\alpha\beta(I-\frac{1}{2}(G_y+G_y{}^T)) > (I+\frac{\beta}{2}N_{yy})(I-\frac{1}{2}(G_y+G_y{}^T))^{-1}(I+\frac{\beta}{2}N_{yy}),$$

which is implied by $\sqrt{\alpha\beta}(1-\rho) > 1+\frac{\beta}{2}\|N_{yy}\|.$

- **Satisfied for** $\beta=\frac{2}{c},\ \alpha=\frac{2c}{(1-\rho)^2}$ **with** $c=\|N_{yy}\|$ **.**

Theorem: **A suitable** B **is given by:**

$$B=\alpha G_u^T G_u+\beta N_{yu}^T N_{yu}+N_{uu}.$$

[Hamdi, Griewank, 2008]

One-step one-shot

Aerodynamic shape design

Descent for $\beta = \frac{2}{c}, \quad \alpha = \frac{2c}{(1-\rho)^2}$ **with** $c = \|N_{yy}\|$ **.**

(In practice choose $c = 1, \;\Rightarrow\; \beta = 2, \;\alpha >> 1.$**)**

A suitable *B* **is given by** $B = \alpha G_u^T G_u + \beta N_{yu}^T N_{yu} + N_{uu}.$

Instead BFGS updates for the Hessian

$$\nabla_u^2 L^a = \underbrace{\alpha G_u^T G_u + \beta N_{yu}^T N_{yu} + N_{uu}}_{B} + \alpha \underbrace{(G - y)}_{\to_* 0}^T G_{uu} + \beta \underbrace{(N_y^T - \bar{y})}_{\to_* 0}^T N_{yuu}.$$

The gradient $\nabla_u L^a = \alpha (G - y)^T G_u + \beta (N_y - \bar{y})^T N_{yu} + N_u$

is evaluated by Algorithmic Differentiation (AD).

One-step one-shot

Aerodynamic shape design

- Transonic case: RAE 2822 at Ma = 0.73 with $\alpha = 2°$
- Cost function: drag (cd)
- TAUij (2D Euler) + mesh deformation + parameterization
- First and second derivatives by AD tool ADOL-C
- Geometric constraint: constant thickness
- Camberline/Thickness decomposition,
  20 Hicks-Henne coefficients define camberline

Automatic Differentiation of Entire Design Chain

design vector (P) $\rightarrow$ defgeo $\xrightarrow{x_{new}}$ difgeo $\xrightarrow{dx}$ meshdefo $\xrightarrow{m}$ flow solver $\rightarrow$ C_D

surface grid $\nearrow$ difgeo; grid $\nearrow$ meshdefo

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

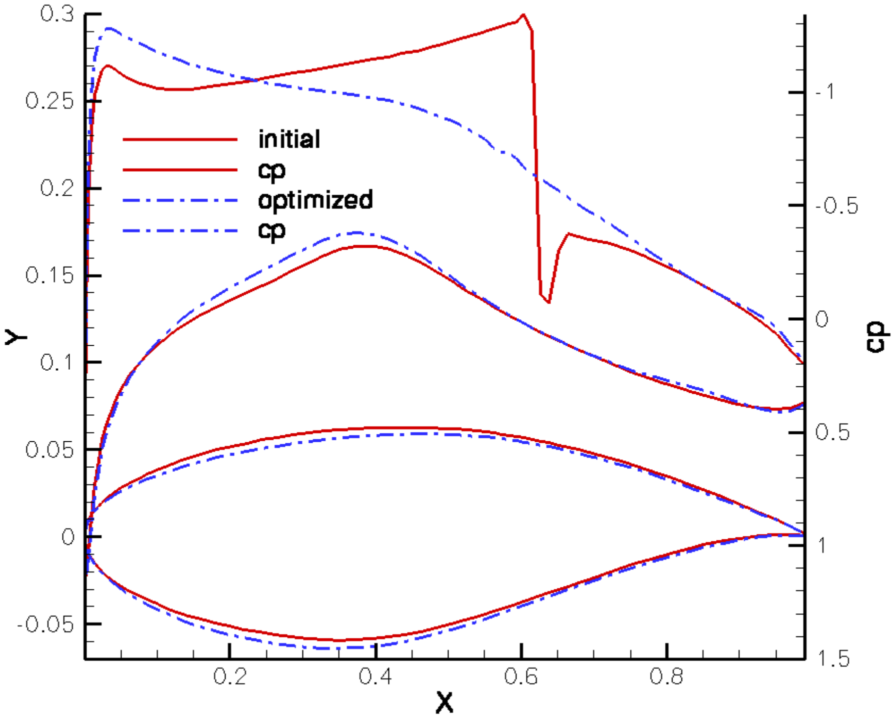
$$\frac{dC_D}{dP} = \frac{\partial C_D}{\partial m} \cdot \frac{\partial m}{\partial (dx)} \cdot \frac{\partial (dx)}{\partial x_{new}} \cdot \frac{\partial x_{new}}{\partial P} \quad \text{and} \quad \frac{\partial (dx)}{\partial x_{new}} = \frac{\partial (x_{new} - x_{old})}{\partial x_{new}} = Id$$

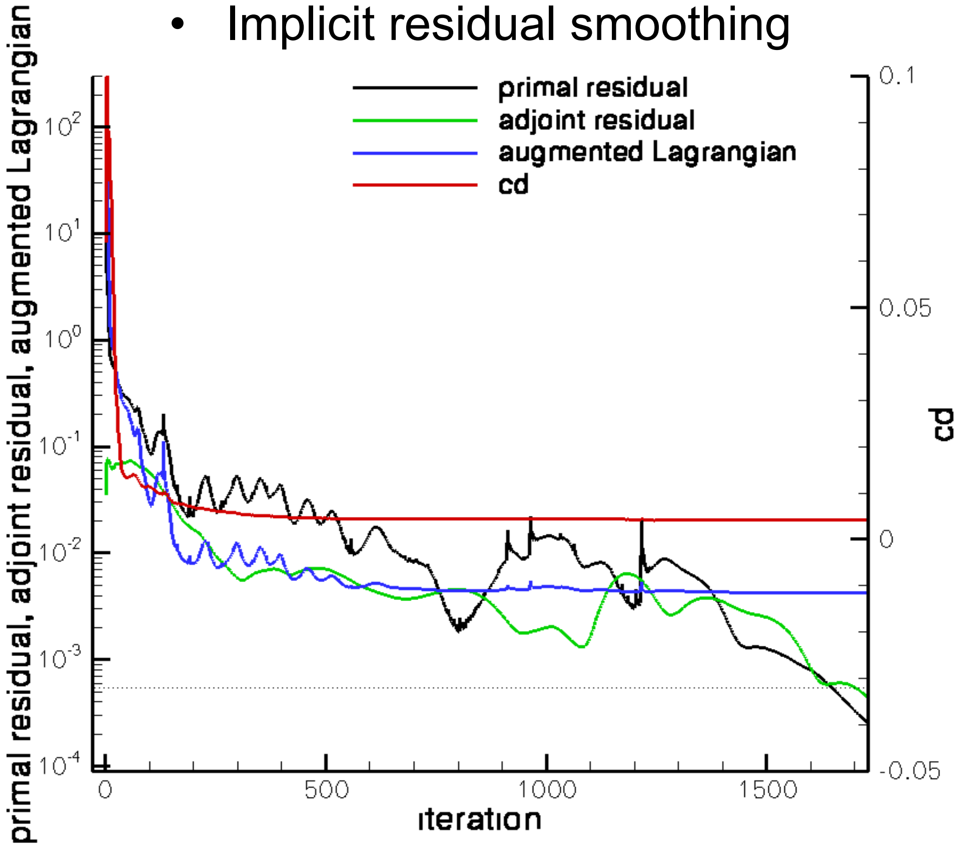
TAUij_AD (↗ ∂m)   meshdefo_AD (↖ $\partial (dx)$)   defgeo_AD (↖ ∂P)

One-step one-shot

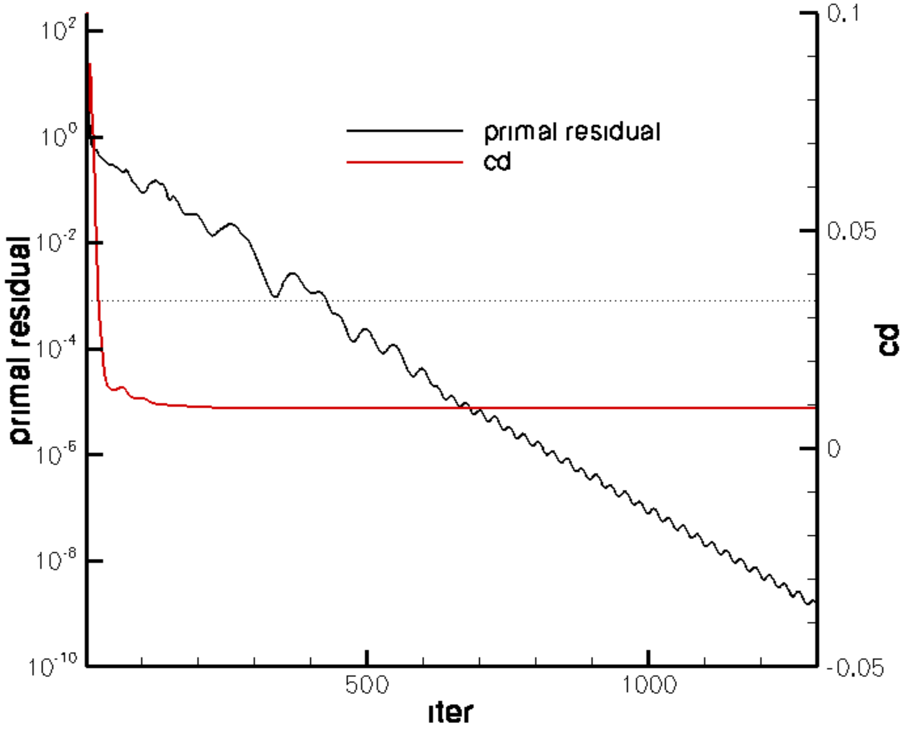
Drag reduction
- RAE 2822, M = 0.73, α = 2.0°
- inviscid flow, mesh 161x33 cells
- 20 design variables (Hicks-Henne)
- One-step one-shot

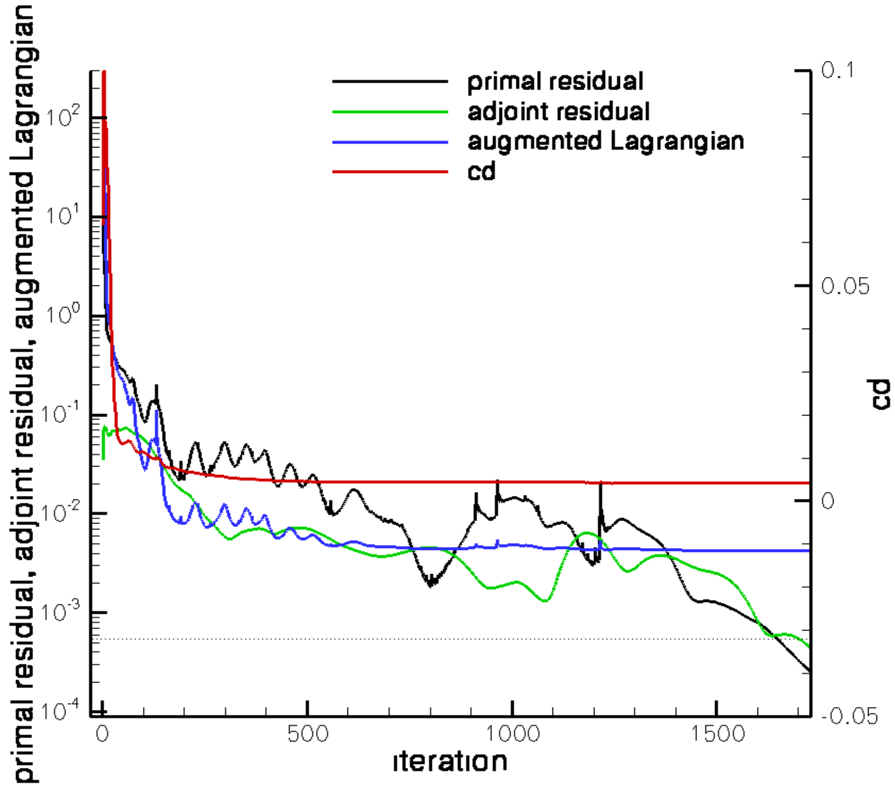
Flow Solver: TAUij
- Compressible Euler
- Explicit RK-4
- Multigrid
- Implicit residual smoothing





Primal compared to coupled iteration





Retardation-Factor = 4

[Özkaya, Gauger, 2008]

Treatment of lift constraint by penalty multiplier method

$$\min_u C_D(y,u) \quad s.t. \quad C_L \geq C_{L,target} \quad and \quad y = G(y,u)$$

Penalty function for lift: $h = (C_{L,target} - C_L), \quad h \overset{!}{\leq} 0$

Redefine objective function: $f = C_D + \lambda h$

$$\min_u C_D(y,u) + \lambda h \quad ; \quad h \rightarrow 0$$

Update the penalty parameter in each one-shot step *k*:

$$\lambda_{k+1} = \lambda_k (1 + ch), \qquad c > 0$$

$$h > 0 \quad \Rightarrow \quad \lambda \uparrow, \qquad h < 0 \quad \Rightarrow \quad \lambda \downarrow$$

A good starting value is: $\lambda_0 = \dfrac{\|\nabla_u C_D\|}{\|\nabla_u h\|}$

Constrained One-Step One-Shot

Drag reduction by constant lift

- RAE 2822, M = 0.73, α = 2.0°
- inviscid flow, mesh 161x33 cells
- 40 design variables (Hicks-Henne)
- One-step one-shot

Flow Solver: TAUij

- Compressible Euler
- Explicit RK-4
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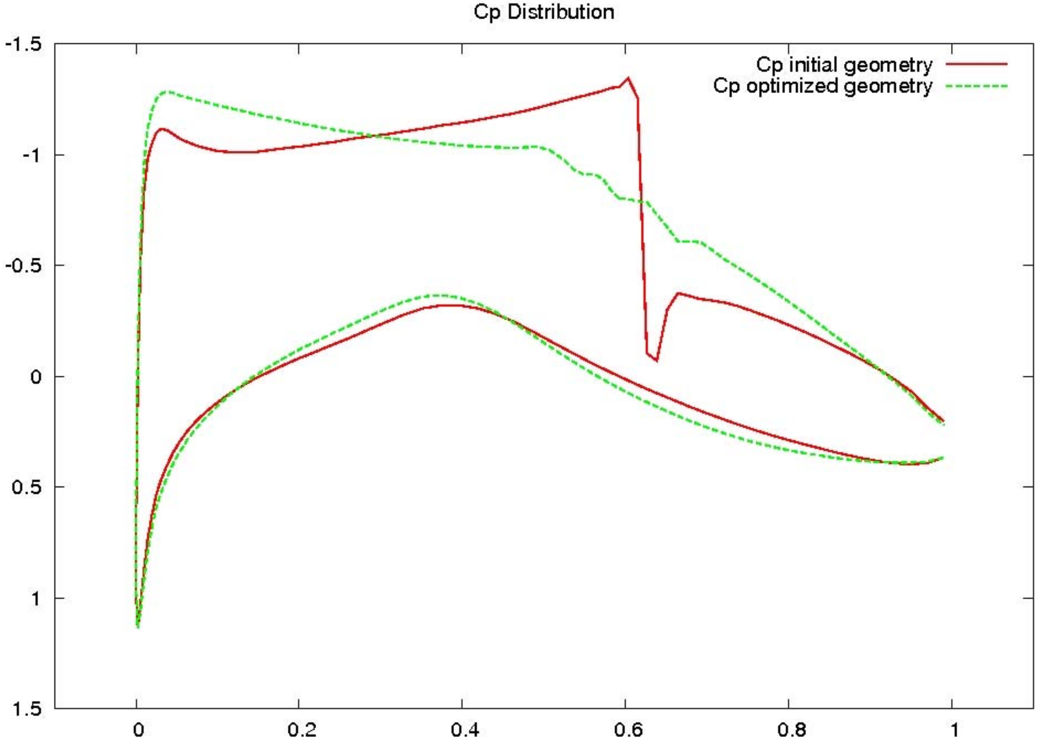
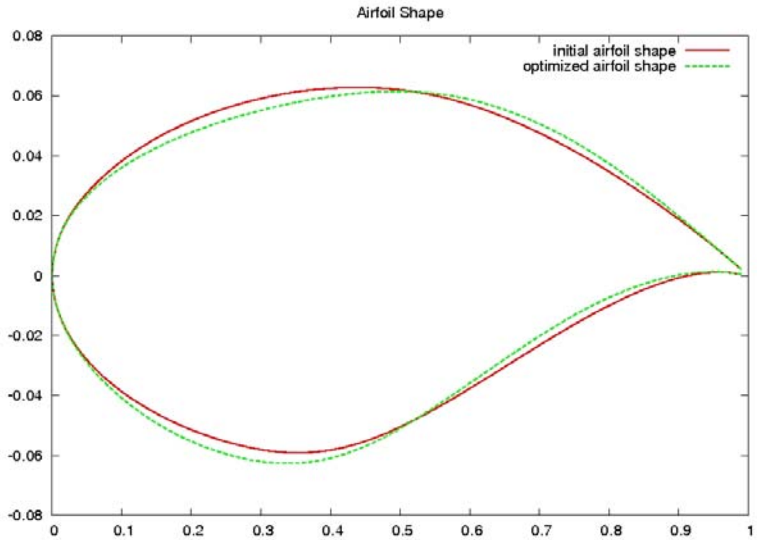
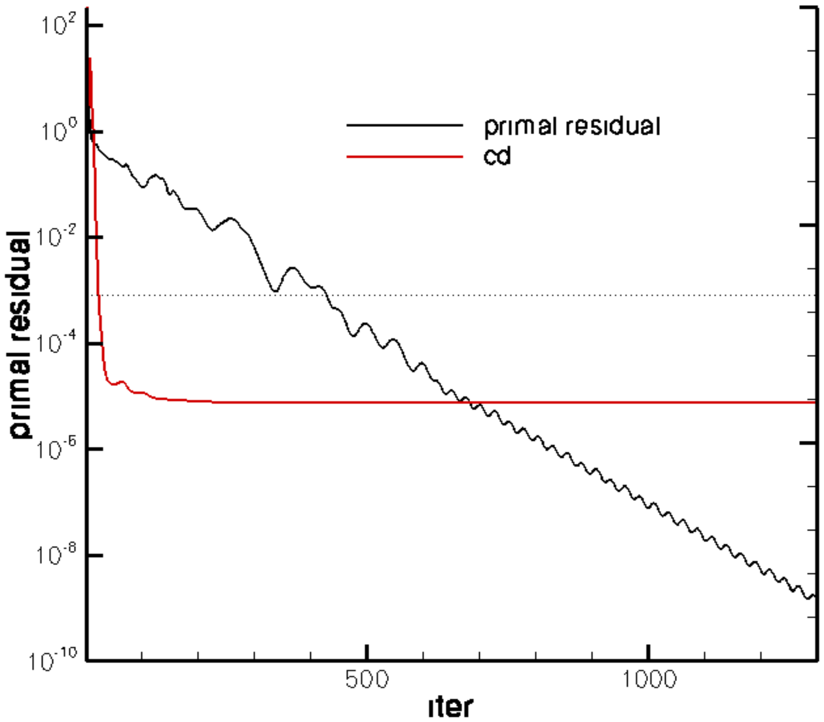
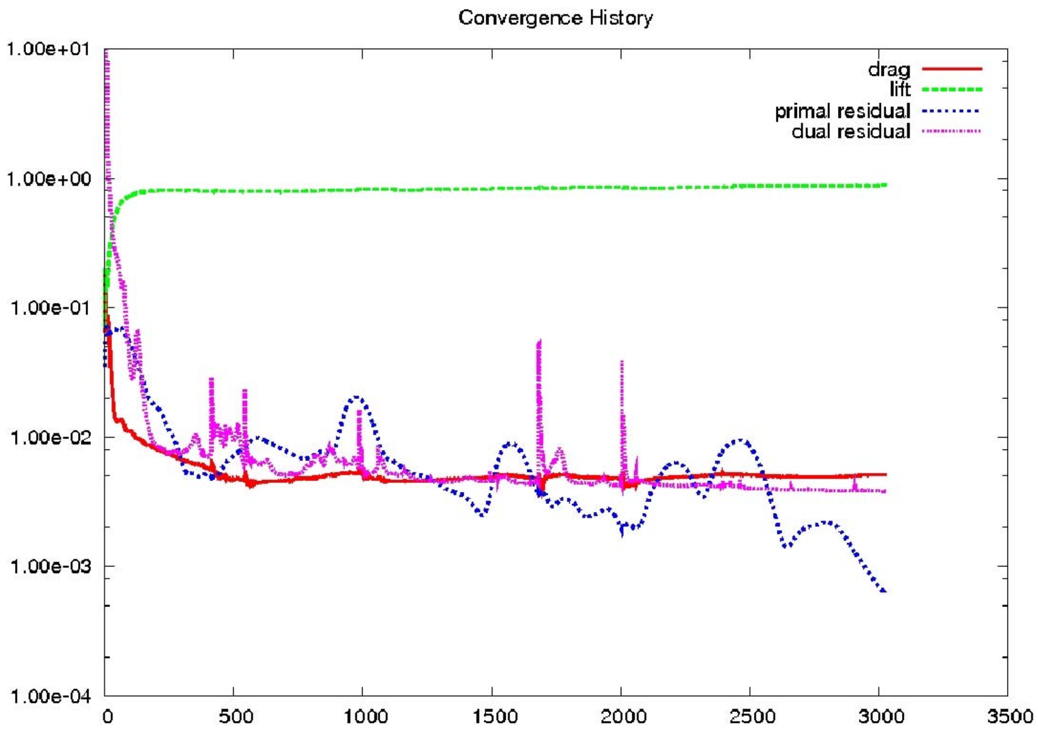
- Implicit residual smoothing





Primal compared to coupled iteration

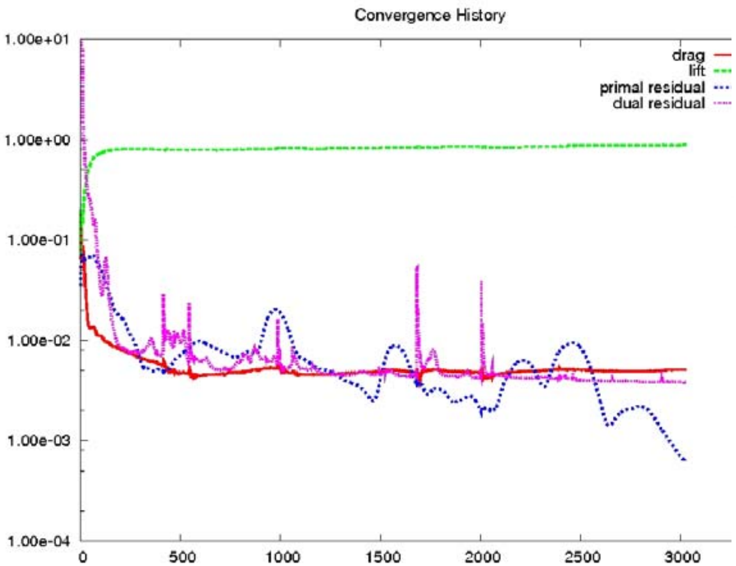


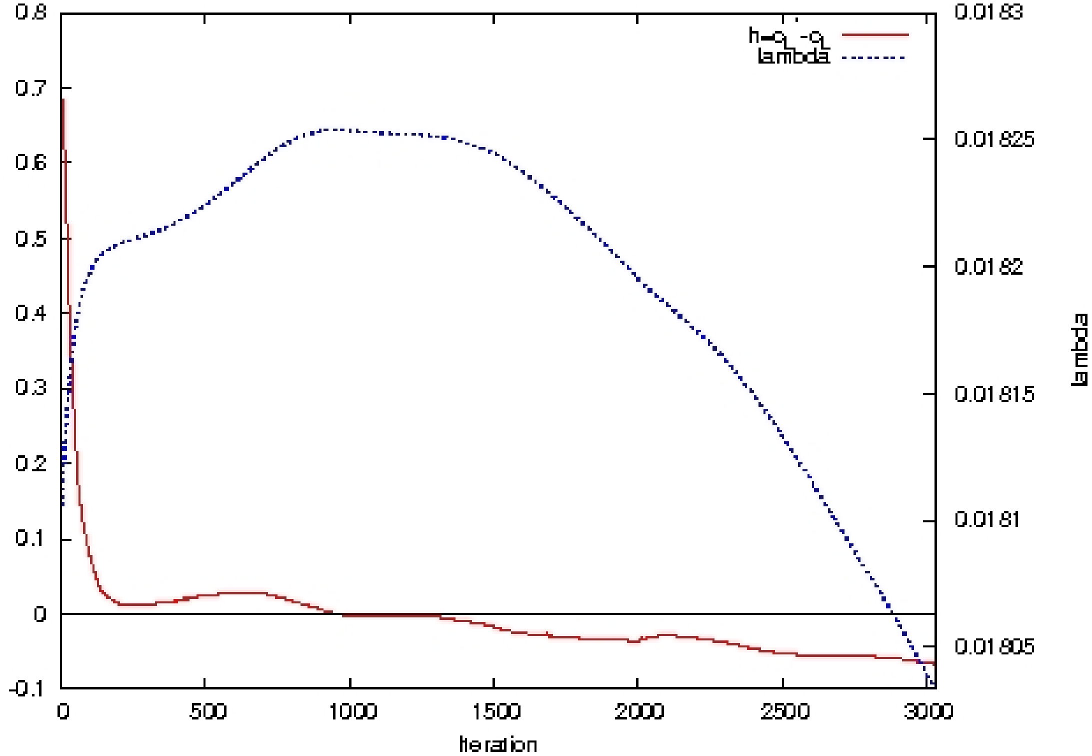


Retardation-Factor = 6

[Gauger, Plocke, 2008]

History of Penalty Multiplier





[Gauger, Plocke, 2008]

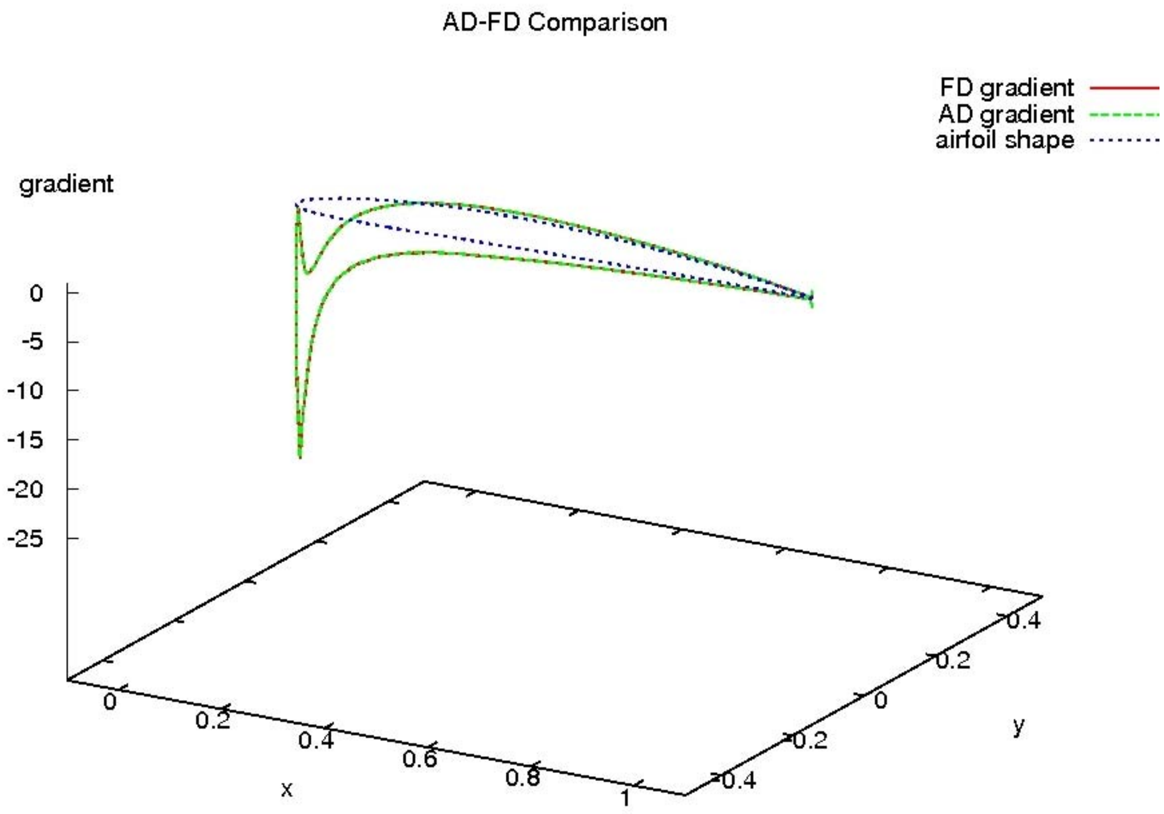
Extension to Navier-Stokes (ELAN Code)

Flow Solver: ELAN (TU Berlin)

- 3D Navier-Stokes (RANS)
- incompressible with pressure correction
- multiblock
- k-ω (Wilcox) turbulence model (and others)
- Fortran (20.000 lines)

AD Tool: TAPENADE (INRIA)

- source to source
- reverse for **first derivatives**
- tangent on reverse for **second derivatives**



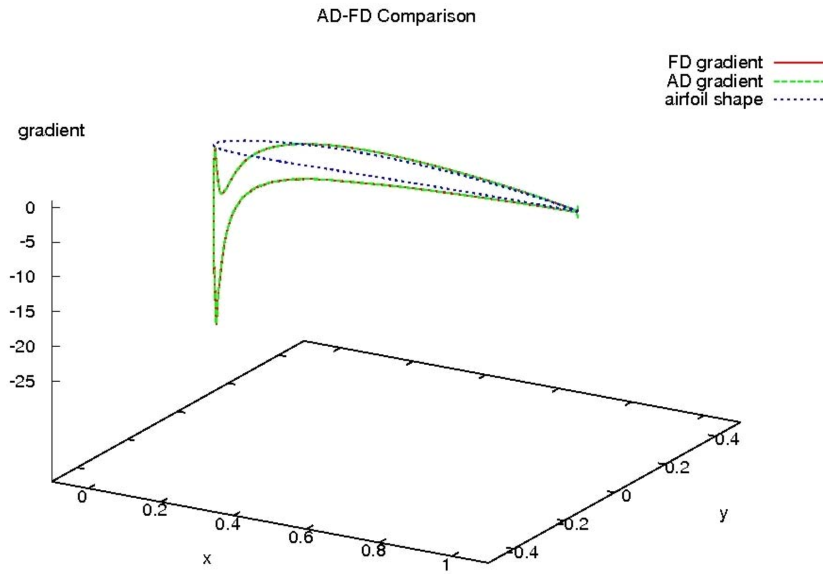
Extension to Navier-Stokes (ELAN Code)

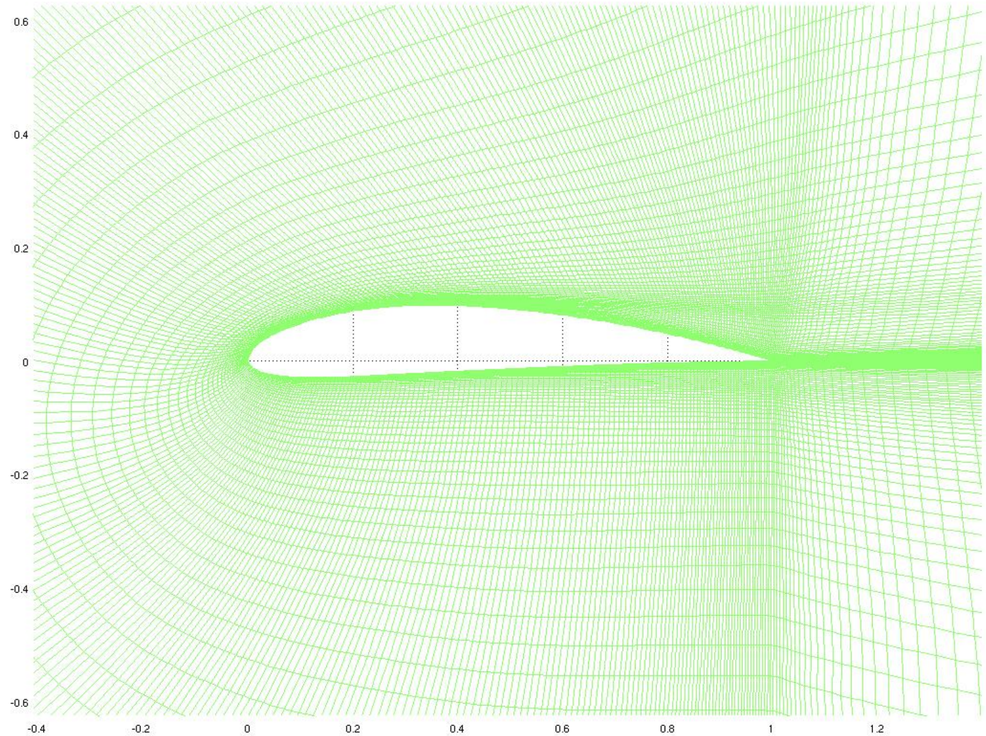
Drag reduction with lift constraint

- NACA 4412
- Re = 1.000.000, α=5.1°
- RANS
- k-ω (Wilcox) turbulence model
- 300 surface mesh points

Approaches for Optimization

- one-shot method
- entire design chain differentiated
- gradient smoothing
- penalty multiplier method





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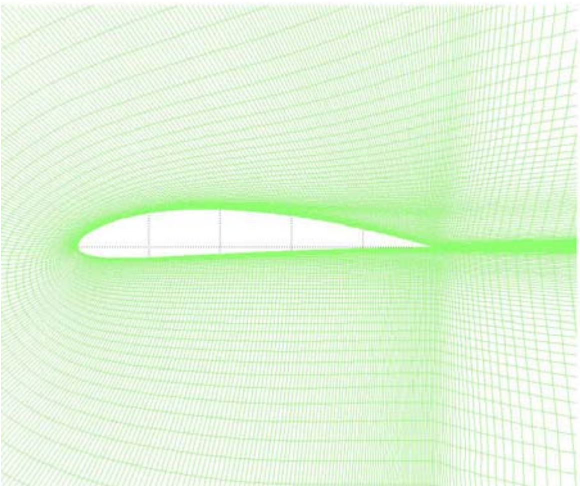

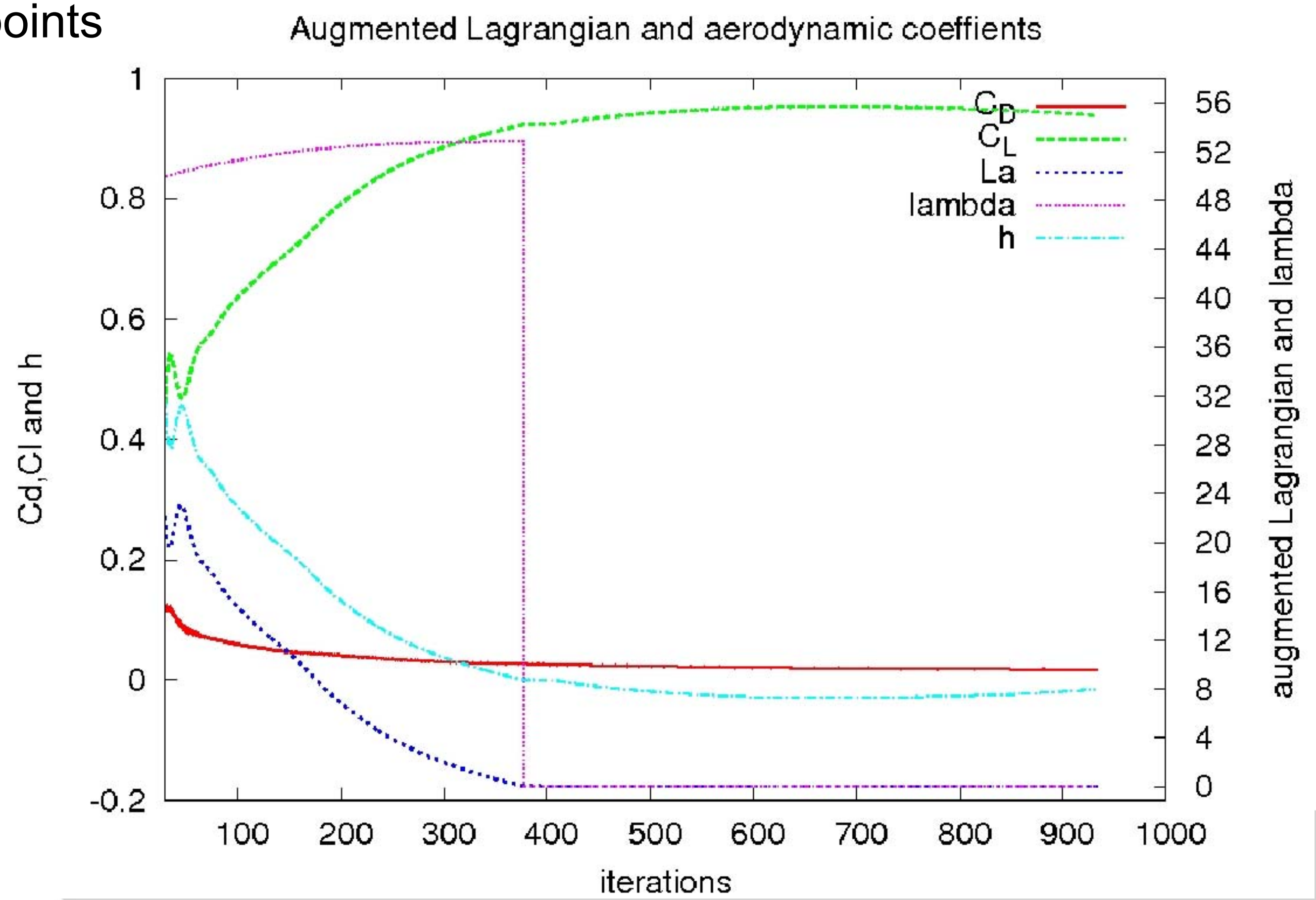

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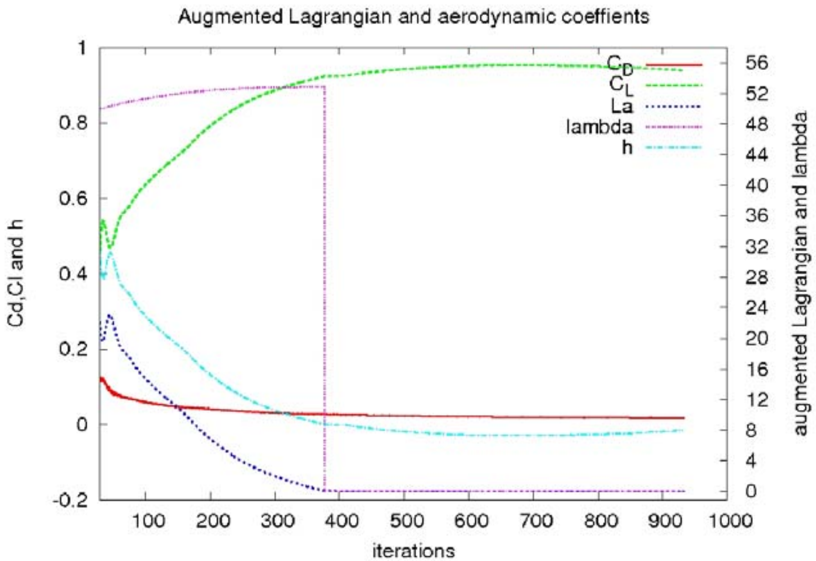
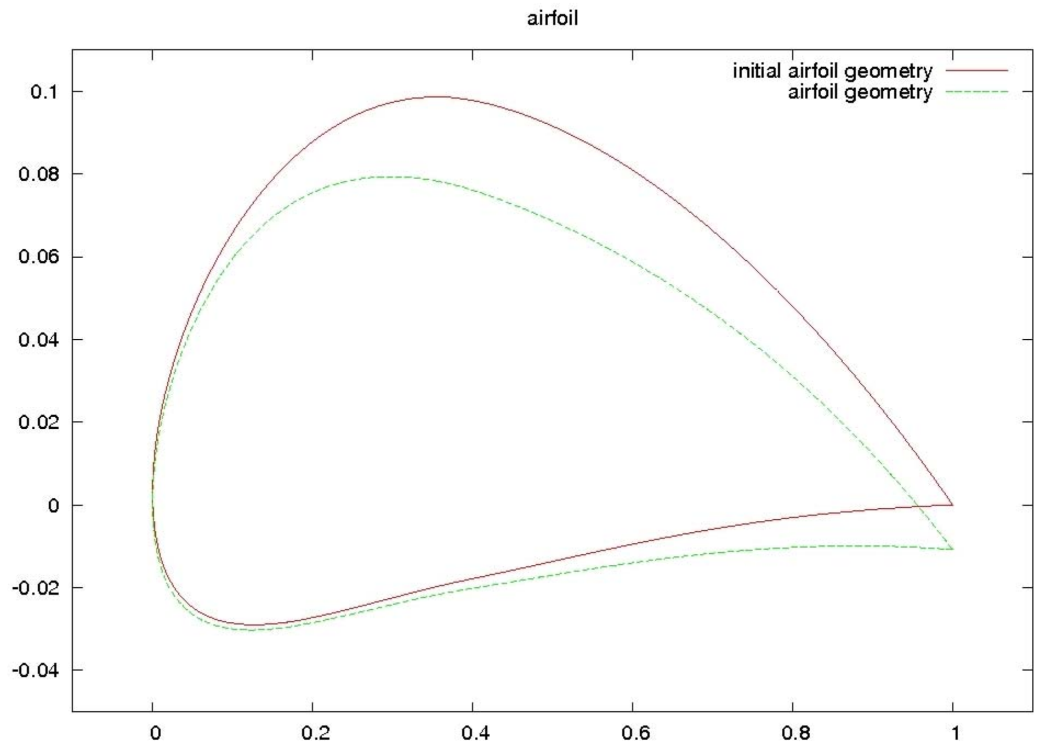
5% drag reduction





[Özkaya, Gauger, 2009]

Thanks for your attention!