Simultaneous Pseudo-Timestepping Methods for Aerodynamic Shape Optimization

Volker Schulz

TEAM: S.B. Hazra (U Trier)
I. Gherman (U Trier)
N. Gauger (DLR)
J. Brezillon (DLR)

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Overview

- Pseudo-timestepping gradient methods
- One-shot strategies
- Choosing a proper design Hessian
- Unconstrained numerical results in 2D
- How to deal with constraints?
- Numerical results in 2D and 3D

Research goal

START: Euler flow (Flower)

based on pseudo timestepping (multigrid)

adjoint pseudo timestepping solver

Goal: ***one-shot algorithm for shape optimization***

Pseudo-timestepping as iterative method

$$Ax = b$$

$$\frac{d}{dt}x(t) = b - Ax(t)$$

$$x^{m+1} = x^m + \lambda\left(b - Ax^m\right)$$

$$\frac{d}{dt}x(t) = W\left(b - Ax(t)\right)$$

$$x^{m+1} = x^m + \lambda W\left(b - Ax^m\right)$$

W is called a preconditioner

steepest descent ps-t.

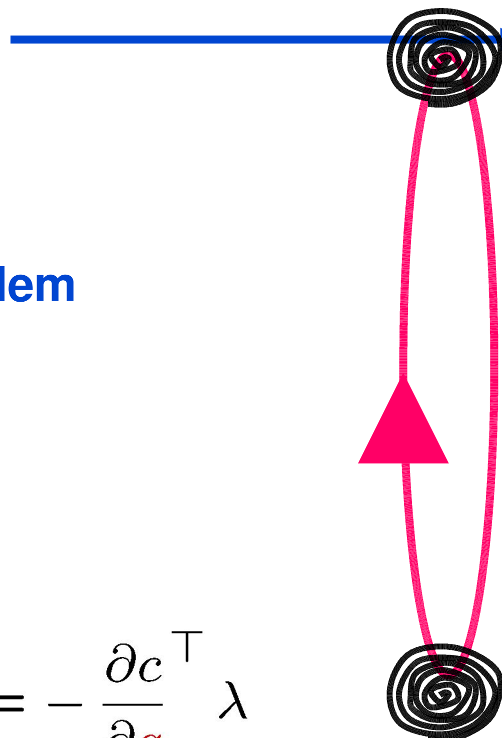
Euler flow

$$c(u) = 0$$

time stepping

$$\dot{u} = -c(u)$$

Flower



optimization problem

$$\min_{q} f(u(q))$$

gradient method

$$q^{k+1} = q^k - \nabla_q f(u(q^k))$$

where

$$\nabla_q f(u(q^k)) = -\frac{\partial c}{\partial q}^\top \lambda$$

with λ from

$$\dot{\lambda} = -\nabla_u \left[f(u, q^k) - \lambda^\top c(u, q^k) \right]$$

Adj. time stepping solver

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One-shot approach

- How to break up the nested iteration loop?
- *Idea:* one pseudo-time loop for all variables

$$\min_{(u,q)} f(u,q) \quad \text{s.t. } c(u,q) = 0 \quad \longrightarrow \quad \begin{aligned} \nabla_u \left[f(u,q) - \lambda^\top c(u,q) \right] &= 0 \\ \nabla_q \left[f(u,q) - \lambda^\top c(u,q) \right] &= 0 \\ c(u,q) &= 0 \end{aligned}$$

One-shot pseudo-time loop

$$\begin{pmatrix} \dot{\lambda} \\ \dot{q} \\ \dot{u} \end{pmatrix} = -\mathbf{W} \begin{pmatrix} \nabla_u \left[f(u,q) - \lambda^\top c(u,q) \right] \\ \nabla_q \left[f(u,q) - \lambda^\top c(u,q) \right] \\ c(u,q) \end{pmatrix}$$

- *W* = *I* leads to slow convergence, if at all
- *W* should improve convergence
- *W* should be „implementation-friendly“
- Borrow *W* from approximate reduced SQP methods

The essence of reduced SQP techniques:

Instead of incrementing by a full SQP method

$$\begin{bmatrix} H_{uu} & H_{uq} & C_u^* \\ H_{qu} & H_{qq} & C_q^* \\ C_u & C_q & 0 \end{bmatrix} \begin{pmatrix} \Delta u \\ \Delta q \\ \Delta \lambda \end{pmatrix} = \begin{pmatrix} -\nabla_u \mathcal{L} \\ -\nabla_q \mathcal{L} \\ -c(u,q) \end{pmatrix}$$

compute increments from

$$\begin{bmatrix} 0 & 0 & C_u^* \\ 0 & B & C_q^* \\ C_u & C_q & 0 \end{bmatrix} \begin{pmatrix} \Delta u \\ \Delta q \\ \Delta \lambda \end{pmatrix} = \begin{pmatrix} -\nabla_u \mathcal{L} \\ -\nabla_q \mathcal{L} \\ -c(u,q) \end{pmatrix}$$

… in pseudo-time-stepping formulation:

$$\begin{pmatrix} \dot{u} \\ \dot{q} \\ \dot{\lambda} \end{pmatrix} = \begin{bmatrix} 0 & 0 & C_u^* \\ 0 & B & C_q^* \\ C_u & C_q & 0 \end{bmatrix}^{-1} \begin{pmatrix} -\nabla_u \mathcal{L} \\ -\nabla_q \mathcal{L} \\ -c(u,q) \end{pmatrix}$$

Use known preconditioners ***A*** for states and adjoints

$$\begin{pmatrix} \dot{u} \\ \dot{q} \\ \dot{\lambda} \end{pmatrix} = \begin{bmatrix} 0 & 0 & A_u^* \\ 0 & B & C_q^* \\ A_u & C_q & 0 \end{bmatrix}^{-1} \begin{pmatrix} -\nabla_u \mathcal{L} \\ -\nabla_q \mathcal{L} \\ -c(u,q) \end{pmatrix}$$

Appropriate *B*?

Options:

- Exact reduced Hessian
- „wrong“ reduced Hessian constructed by use of the state preconditioner

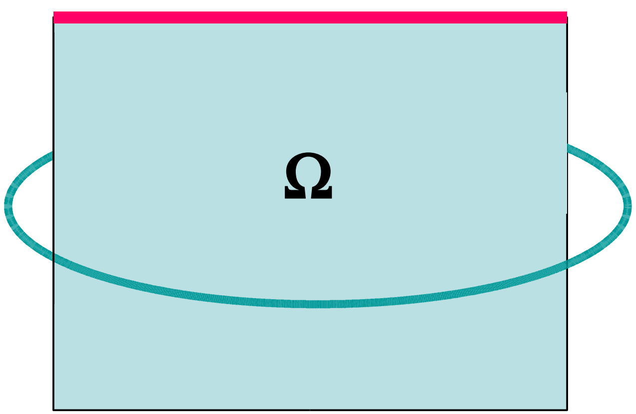
  (cf. Bank/Welfert/Yserentant: A class of iterative methods for solving saddle point problems, Numer. Math. 56, 645-666, 1990)

- Griewank‘s *H(-1)*

Model problem

$$\min_{u,q} \int_{y=1} \left(\frac{\partial u}{\partial \eta} - g(x) \right)^2 dx + \sigma \|q\|_{H^1}^2$$

$$\text{s.t.} \quad \begin{aligned} -\triangle u &= 0 \text{ in } \Omega \\ u &= q(x) \text{ on } y = 1 \\ u &= u_0 \text{ on } y = 0 \end{aligned}$$



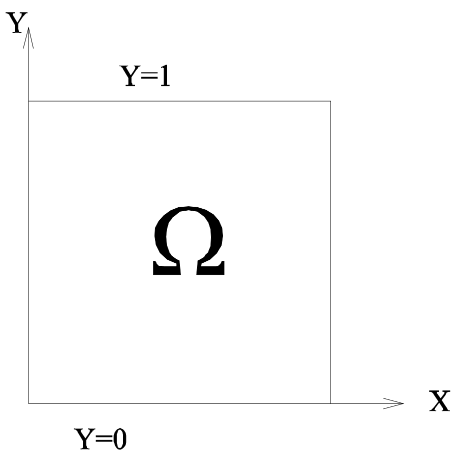
Elliptic PDE to be solved by a pseudo-timestepping method with RK4

Necessary condition $\Rightarrow$

$$-\Delta\lambda = 0 \quad \text{in } \Omega$$

(Costate) $$\lambda + 2\left(\frac{\partial u}{\partial \eta} - g(x)\right) = 0 \quad \text{on } y = 1$$

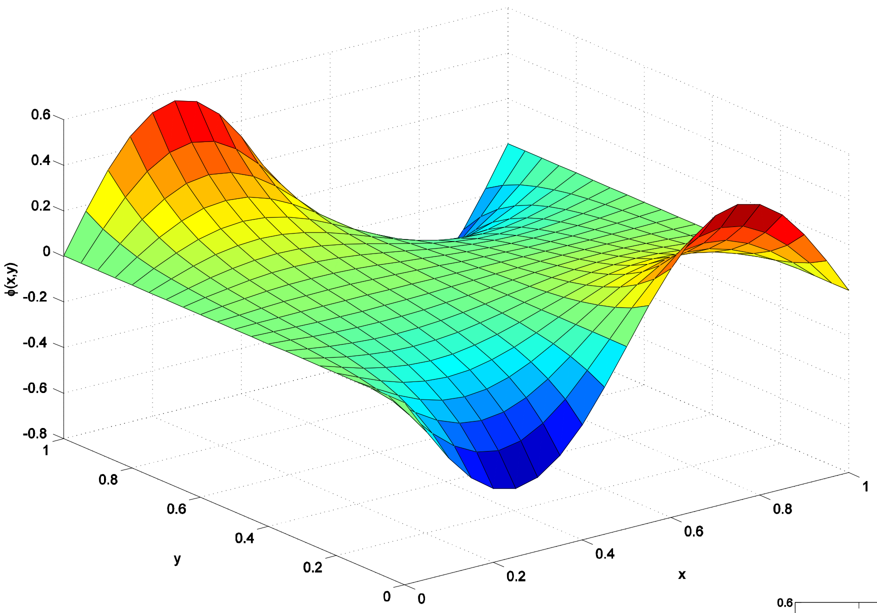
$$\lambda = 0 \quad \text{on } y = 0$$

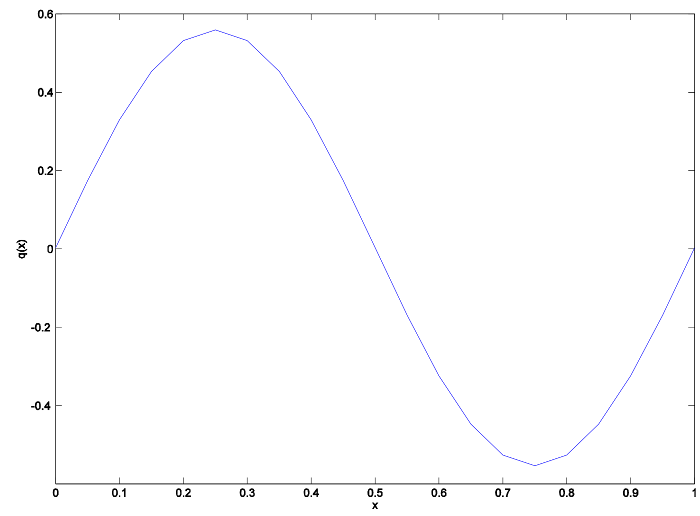


and

(Design) $$2\sigma\left(I - \Delta\right) q - \frac{\partial \lambda}{\partial \eta} = 0 \quad \text{on } y = 1.$$

Solution


0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
ϕ(x,y)
1
0.8
0.6
0.4
0.2
0
y
0
0.2
0.4
0.6
0.8
1
x


0.6
0.4
0.2
0
-0.2
-0.4
q(x)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x

Pseudo-time embedding (unpreconditioned)

$$\frac{d\phi}{dt} - \Delta\phi = 0 \quad \text{in} \quad \Omega$$

$$\frac{d\phi}{dt} + \phi - q(x) = 0 \quad \text{on} \quad y = 1$$

$$\frac{d\phi}{dt} + \phi - \phi_0 = 0 \quad \text{on} \quad y = 0$$

$$\frac{d\lambda}{dt} - \Delta\lambda = 0 \quad \text{in} \quad \Omega$$

$$\frac{d\lambda}{dt} + \lambda + 2\left(\frac{\partial\phi}{\partial\eta} - g(x)\right) = 0 \quad \text{on} \quad y = 1$$

$$\frac{d\lambda}{dt} + \lambda \qquad\qquad = 0 \quad \text{on} \quad y = 0$$

$$\frac{dq}{dt} + 2\sigma q - \frac{\partial\lambda}{\partial\eta} = 0 \quad \text{on} \quad y = 1 \;.$$

What about the reduced Hessian approximation *B*?

- Interpretation as pseudo-differential operator whose symbol can be investigated analytically

- Application of calculus of variations

Both lead to the result:

$$B = 2(\sigma I - (1+\sigma)\frac{\partial^2}{\partial x^2})$$

A closer look at the RSQP-matrix

Instead of

$$\begin{pmatrix} \dot{u}_i \\ \dot{u}_b \\ \dot{q} \\ \dot{\lambda}_b \\ \dot{\lambda}_i \end{pmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 & -\triangle \\ 0 & 0 & 0 & I & L_b^* \\ 0 & 0 & B & -I & 0 \\ 0 & I & -I & 0 & 0 \\ -\triangle & L_b & 0 & 0 & 0 \end{bmatrix}^{-1} \begin{pmatrix} -\nabla_{u_i}\mathcal{L} \\ -\nabla_{u_b}\mathcal{L} \\ -\nabla_q\mathcal{L} \\ -c_b \\ -c_i \end{pmatrix}$$

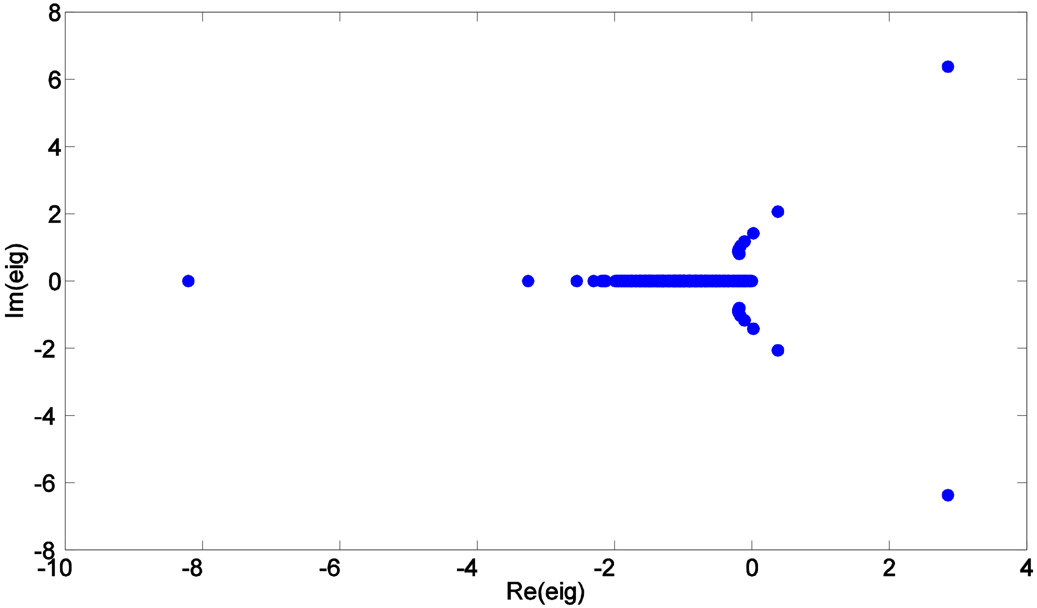
we use

$$\begin{pmatrix} \dot{u}_i \\ \dot{u}_b \\ \dot{q} \\ \dot{\lambda}_b \\ \dot{\lambda}_i \end{pmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 & -D \\ 0 & 0 & 0 & I & L_b^* \\ 0 & 0 & D_B & -I & 0 \\ 0 & I & -I & 0 & 0 \\ -D & L_b & 0 & 0 & 0 \end{bmatrix}^{-1} \begin{pmatrix} -\nabla_{u_i}\mathcal{L} \\ -\nabla_{u_b}\mathcal{L} \\ -\nabla_q\mathcal{L} \\ -c_b \\ -c_i \end{pmatrix}$$

First Test

- *D* is diagonal of Laplacian (Jacobi prec)
- *B* is exact reduced Hessian
- One-shot pseudo-time integration by classical RKF45

Eigenvalues of resulting dynamical system – <u>no convergence</u>

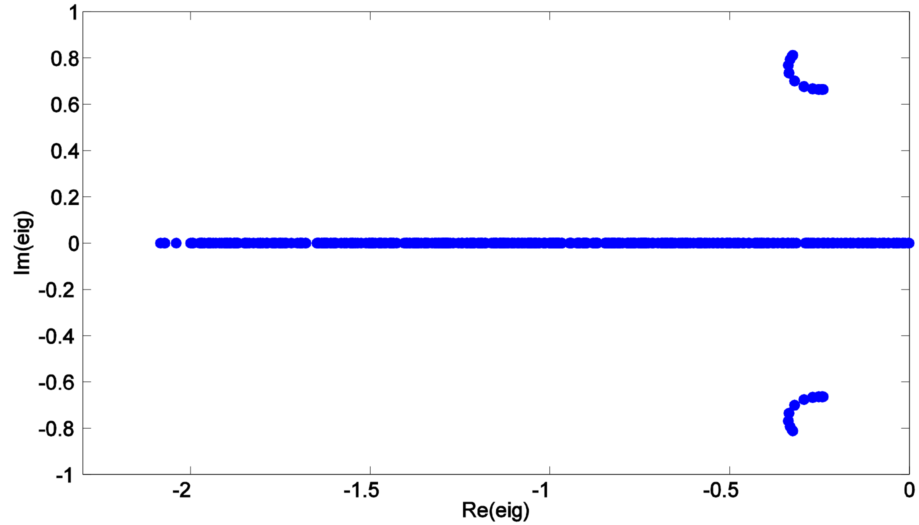


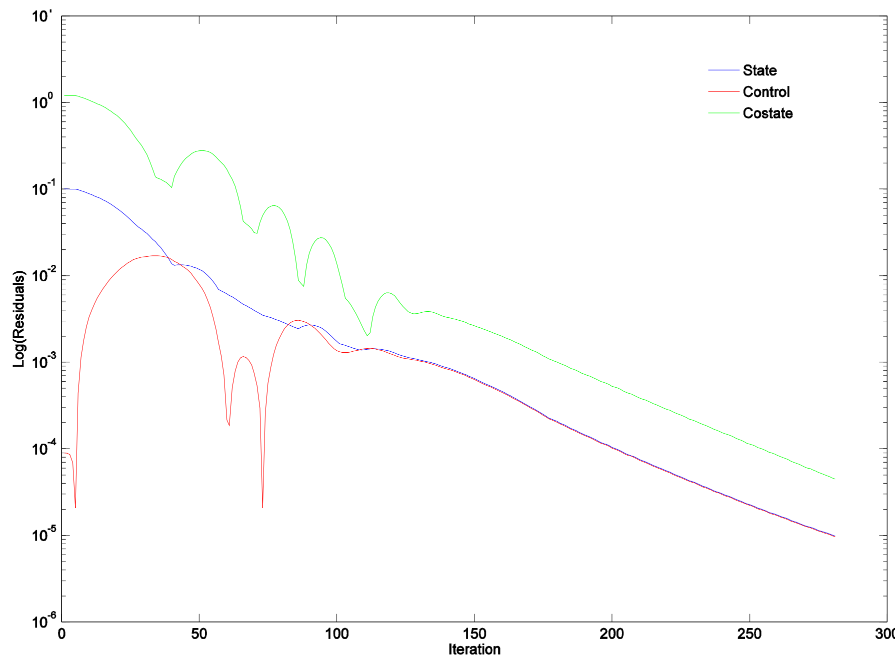
Second Test

- *D* is diagonal of Laplacian (Jacobi prec)
- *B* is „wrong“ reduced Hessian

  (built by the use of *D* instead of Laplacian)

Eigenvalues of resulting dynamical system – <u>convergence</u>





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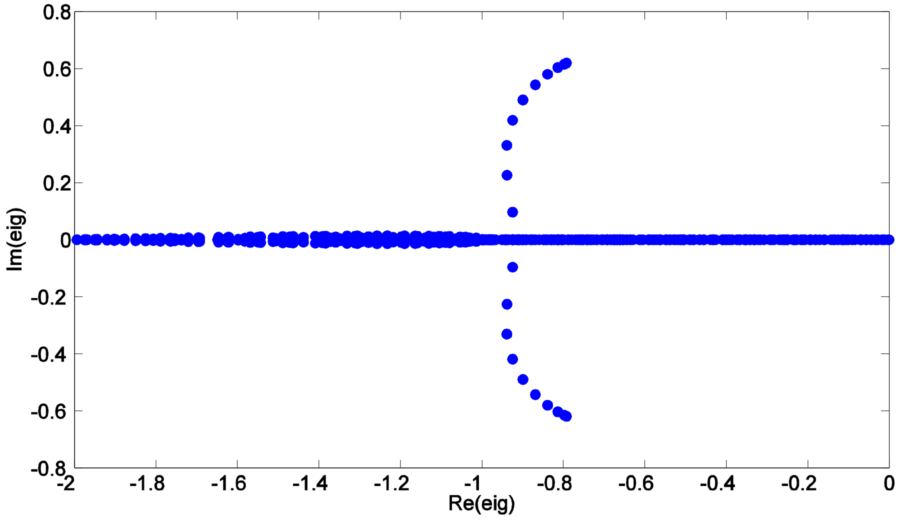
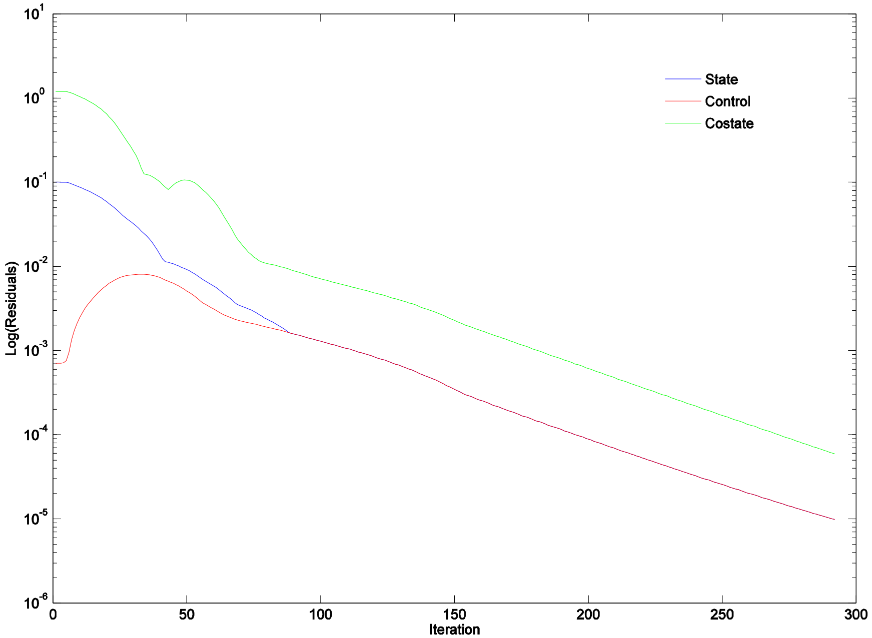
3rd Test

Eigenvalues of resulting dynamical system – <u>convergence</u>

- *D* is diagonal of Laplacian (Jacobi prec)
- *B* is diagonal of exact Hessian



$$\frac{\text{optimization effort}}{\text{state effort}} < 4$$



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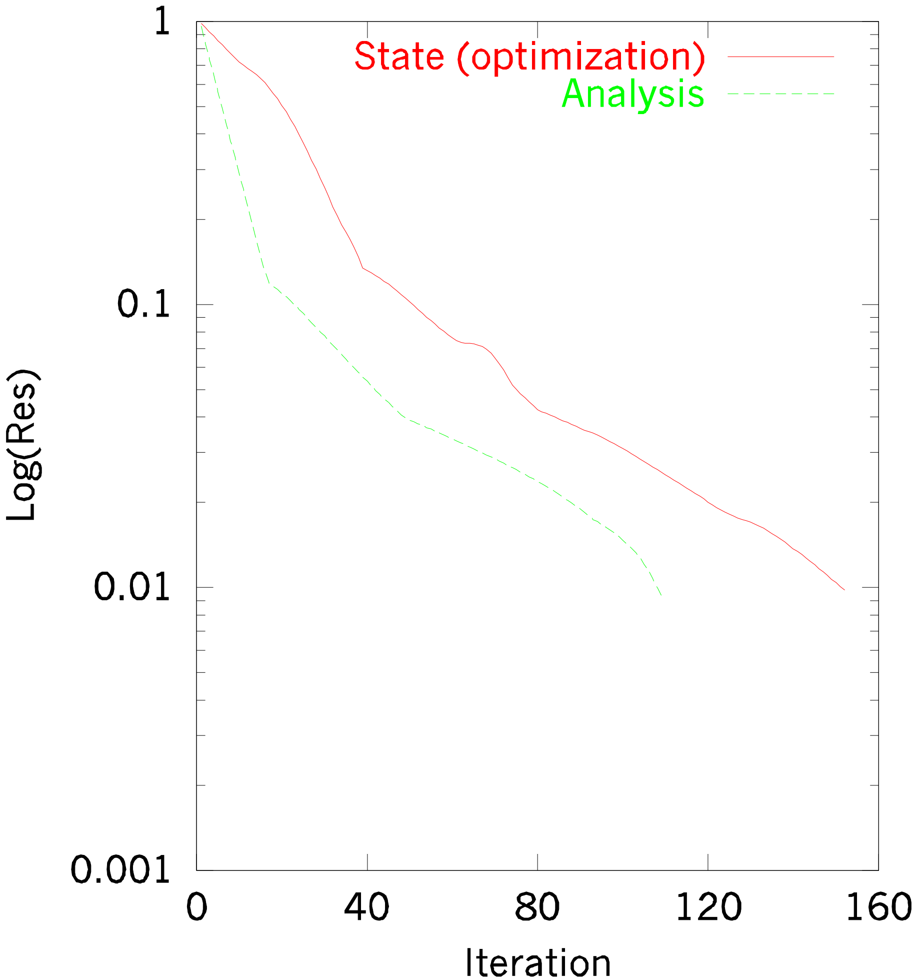
consequences

- 4th test with D=Laplacian and exact reduced Hessian yields also convergence but by a tremendous computational effort
- ***We conclude*** that reduced Hessian approximation should be constructed consistent with forward preconditioner
- Too much effort in producing the exact reduced Hessian is wasted.

Numerical result for 20x20 finite difference discretization: overall Runge-Kutta integration



one-shot optimization

$$\frac{\text{optimization effort}}{\text{state effort}} < 4$$

→ *Without preconditioning factor 1000 !*

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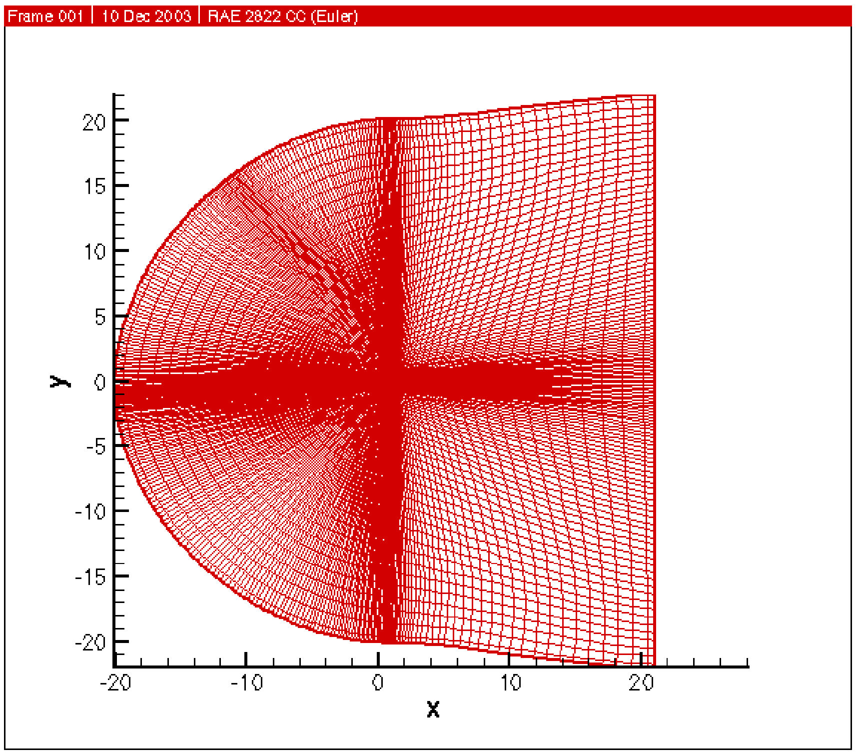
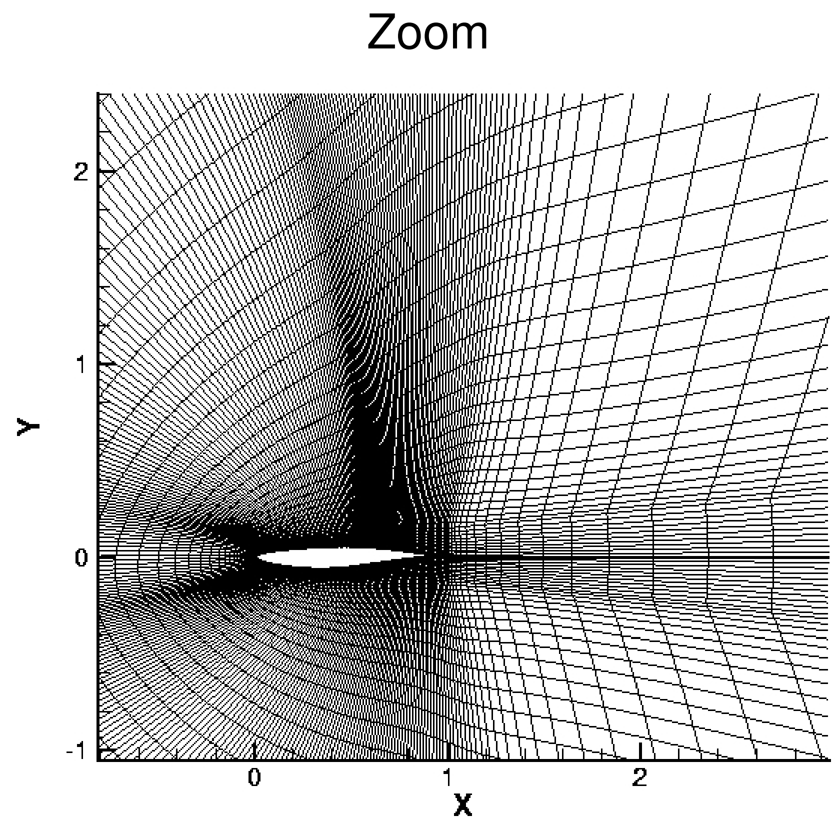
Minimize Drag of an RAE 2822 airfoil by use of *Flower*/DLR within rSQP one shot optimization





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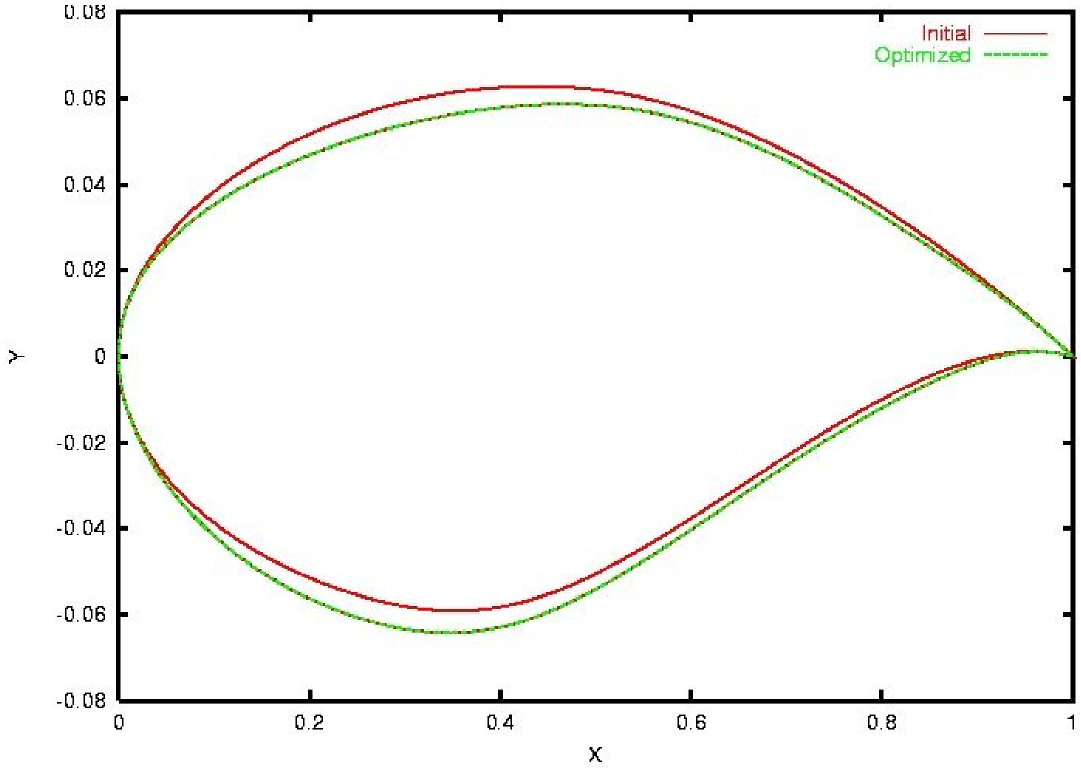
2D-results

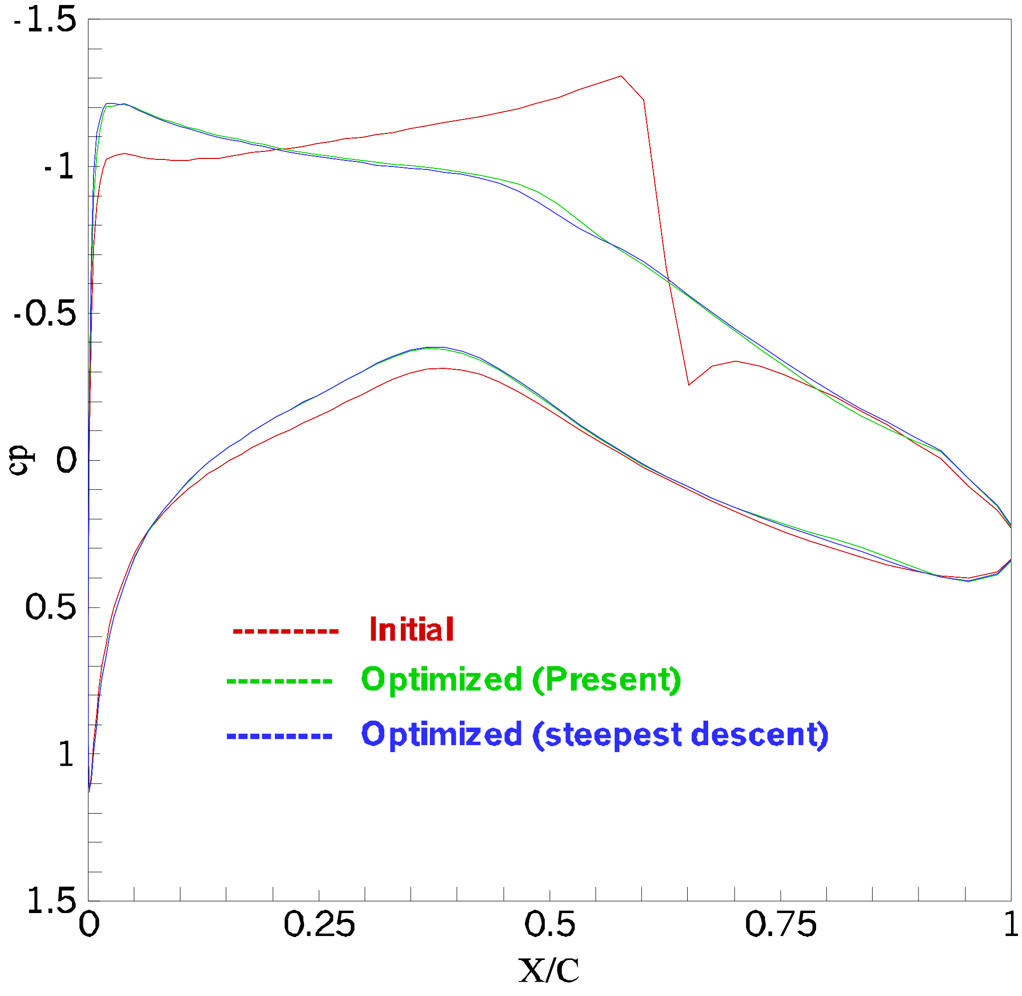
- Euler flow (Code: *Flower*/DLR) with adjoint solver by Gauger
- Minimize drag subject to constant profile thickness: 66% reduction achieved
- Technique employed per iteration:
  - State/adjoint: single RK-steps provided by *Flower*
  - Design: explicit Euler with scalar reduced Hessian approximation of the form: $B \approx \frac{(\gamma^k - \gamma^{k-1})^\top \Delta q^k}{\|\Delta q^k\|^2} \cdot I$

where $\gamma^k = \nabla_q f^k - C_q^\top \lambda^k \approx \text{"reduced gradient"}$

Profile change



Pressure over profile length



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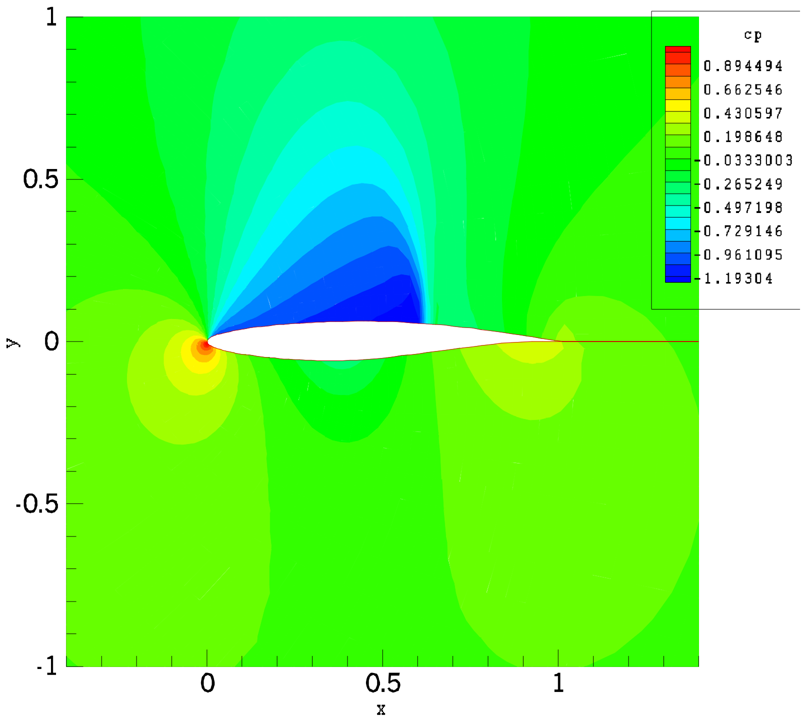
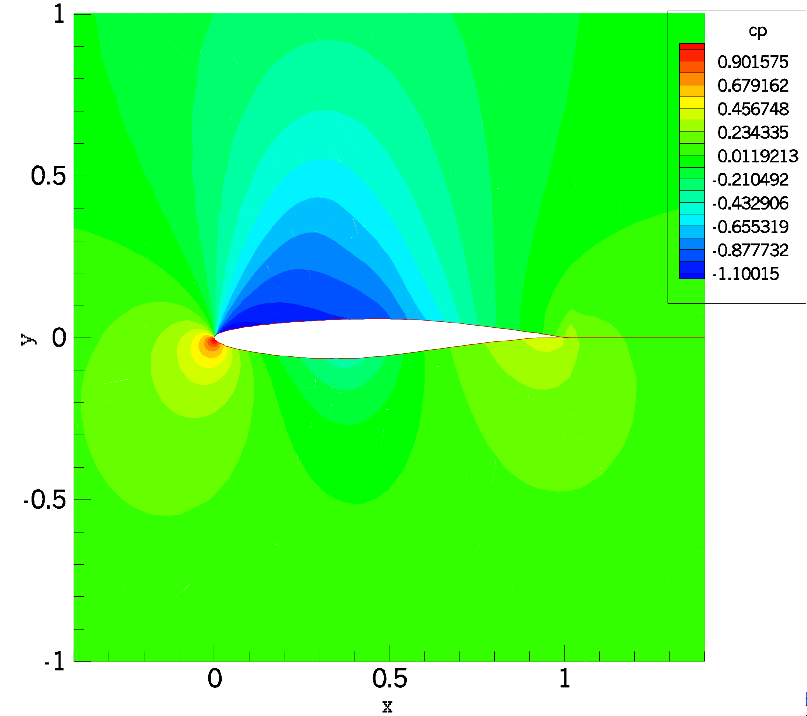
Pressure

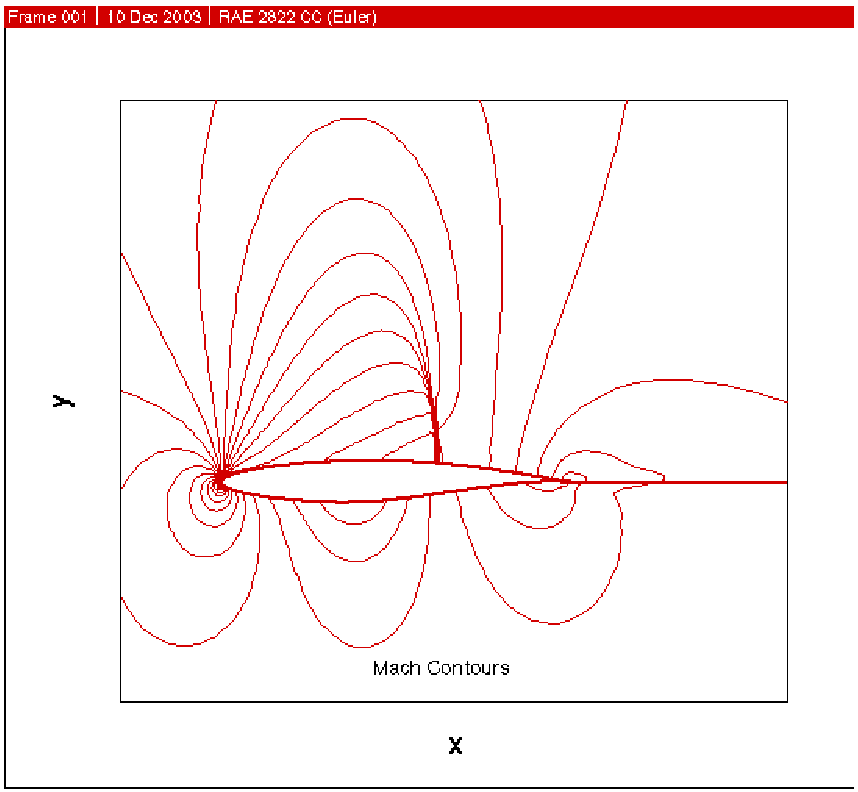
before opt

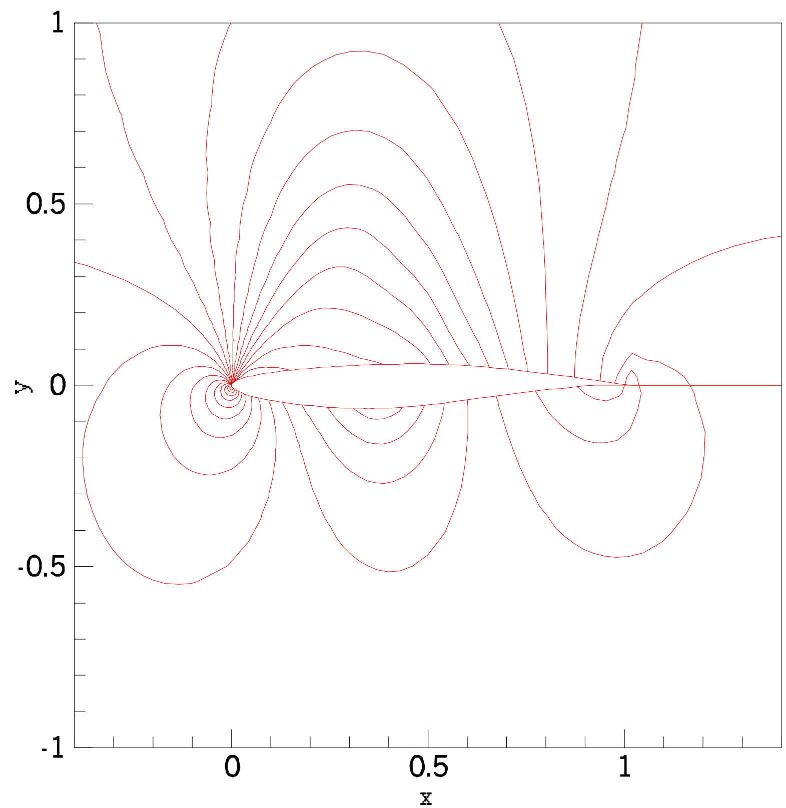


after opt

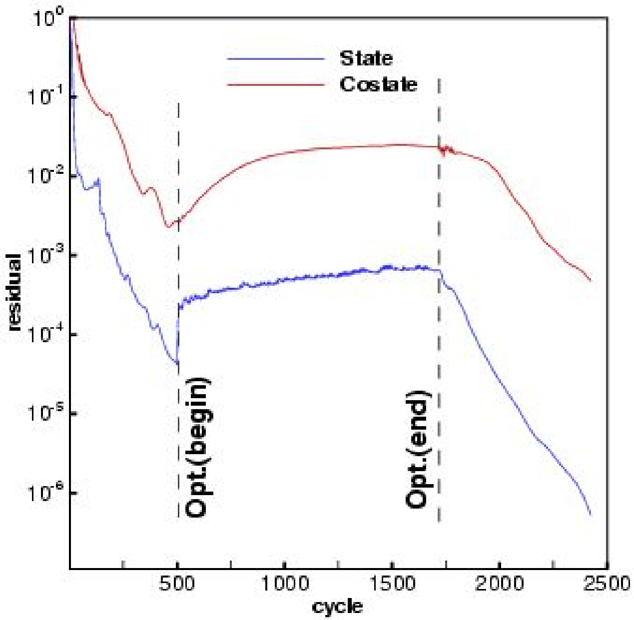


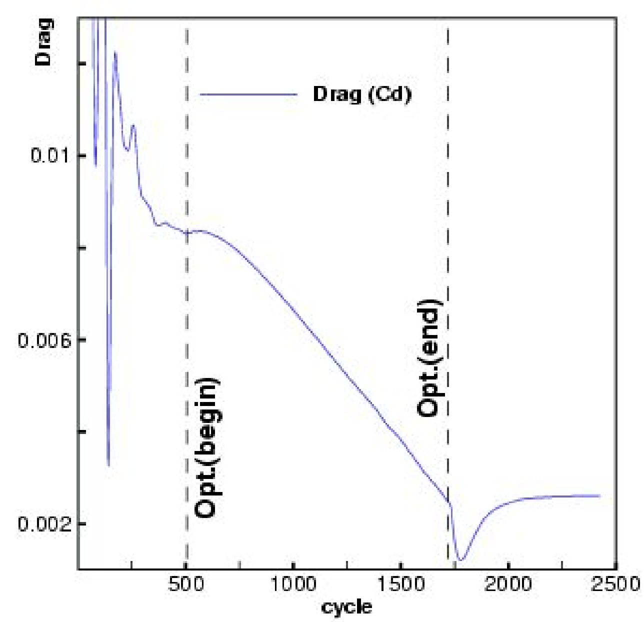
Mach number (velocity)





Convergence history

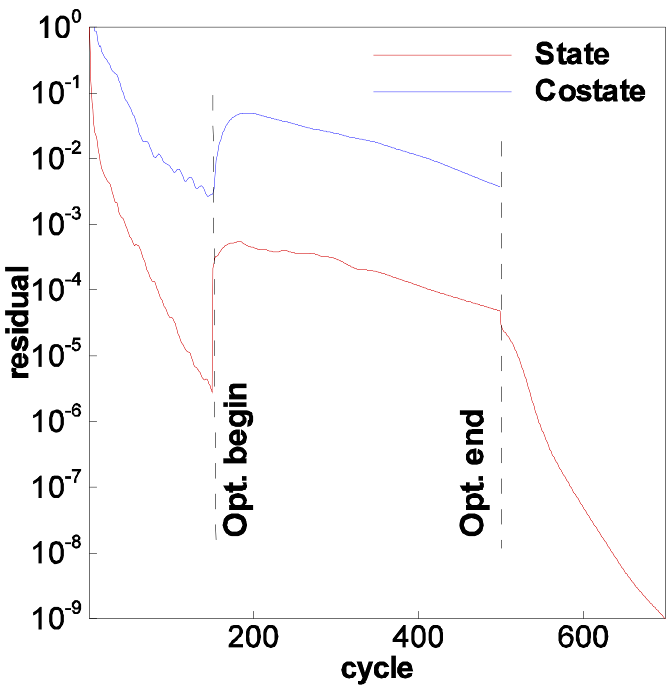


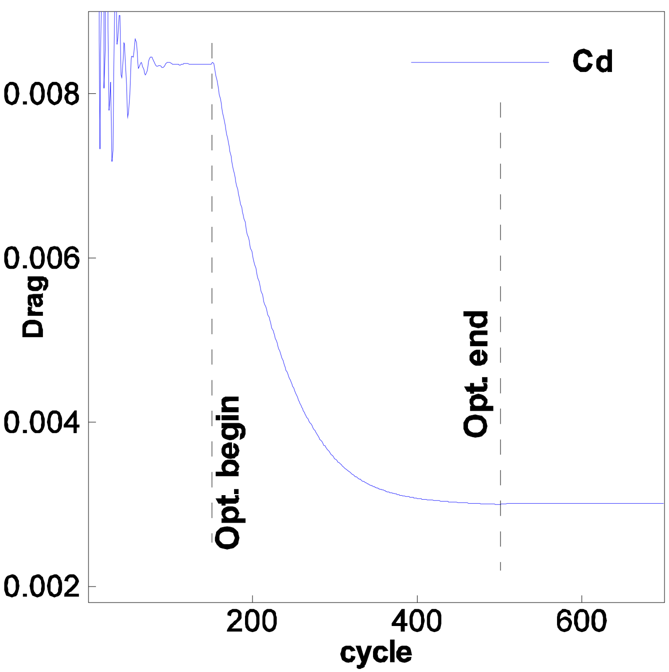


One forward run requires 1500 iterations

$$\Rightarrow \frac{\text{optimization effort}}{\text{state effort}} < 4$$

Multigrid results
(3 grid levels)





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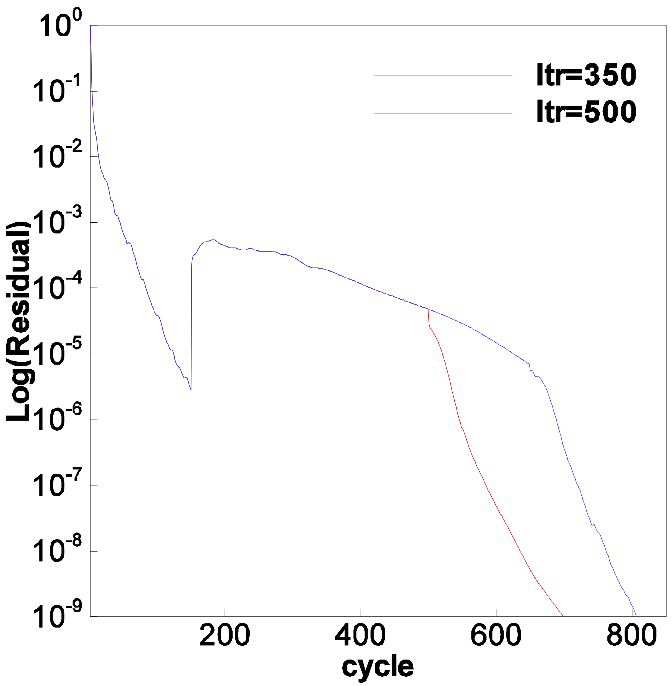
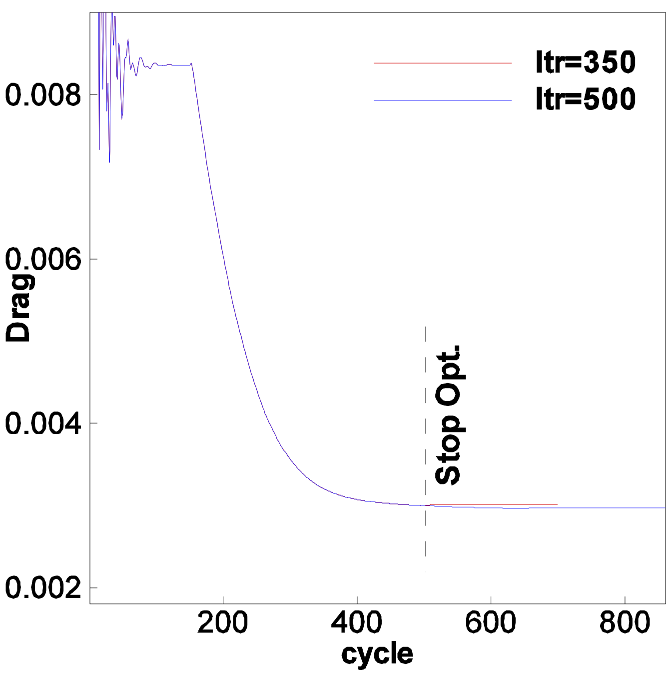
Iterating to „infinity"





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State constraints

Real goal:

minimize **drag**

s.t. **lift >= $\underline{l}$**

where **lift: (u,q) R^1**

depends on the states and can be computed by the solution of yet another adjoint problem!

(no adjustment of angle of incidence)

Algorithmic extension

$$\min_{u,q} f(u,q)$$
$$\text{s.t.} \quad h(u,q) \geq h_0 \quad \in R^1$$
$$c(u,q) = 0, \quad \exists c_u^{-1}$$

Newton-KKT

$$\begin{bmatrix} H_{uu} & H_{uq} & h_u^* & C_u^* \\ H_{qu} & H_{qq} & h_q^* & C_q^* \\ h_u & h_q & 0 & 0 \\ C_u & C_q & 0 & 0 \end{bmatrix} \begin{pmatrix} \Delta u \\ \Delta q \\ \Delta \mu \\ \Delta \lambda \end{pmatrix} = \begin{pmatrix} -\nabla_u \mathcal{L} \\ -\nabla_q \mathcal{L} \\ -h(u,q) \\ -c(u,q) \end{pmatrix}$$

is substituted by time-evolution

$$\begin{bmatrix} 0 & 0 & 0 & D_u^* \\ 0 & B & \tilde{\gamma}^* & C_q^* \\ 0 & \tilde{\gamma} & 0 & 0 \\ D_u & C_q & 0 & 0 \end{bmatrix} \begin{pmatrix} \dot{u} \\ \dot{q} \\ \dot{\mu} \\ \dot{\lambda} \end{pmatrix} = \begin{pmatrix} -\nabla_u \mathcal{L} \\ -\nabla_q \mathcal{L} \\ -h(u,q) \\ -c(u,q) \end{pmatrix}$$

Where $\tilde{\gamma}$ denotes the current gradient approximation from adjoint lift time-evolution

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One approximate Newton step for the constraint problem:

$$\begin{pmatrix} 0 & 0 & \left(\frac{\partial h}{\partial w}\right)^\top & A^\top \\ 0 & B & \left(\frac{\partial h}{\partial q}\right)^\top & \left(\frac{\partial c}{\partial q}\right)^\top \\ \frac{\partial h}{\partial w} & \frac{\partial h}{\partial q} & 0 & 0 \\ A & \frac{\partial c}{\partial q} & 0 & 0 \end{pmatrix} \begin{pmatrix} \Delta w \\ \Delta q \\ \Delta \mu \\ \Delta \lambda \end{pmatrix} = \begin{pmatrix} -\nabla_w L \\ -\nabla_q L \\ -h \\ -c \end{pmatrix}.$$

„Partially reduced SQP method“

Block-Gauss-reduction to:

$$\begin{pmatrix} B & g_h \\ g_h^\top & 0 \end{pmatrix} \begin{pmatrix} \Delta q \\ \Delta \mu \end{pmatrix} = \begin{pmatrix} -\nabla_q L + \left(\frac{\partial c}{\partial q}\right)^\top A^{-\top} \nabla_w L \\ -h + \frac{\partial h}{\partial w} A^{-1} c \end{pmatrix},$$

with the reduced gradient

$$g_h := \left(\frac{\partial h}{\partial q} - \frac{\partial h}{\partial w} A^{-1} \frac{\partial c}{\partial q} \right)^\top = \begin{bmatrix} -A^{-1} \frac{\partial c}{\partial q} \\ I \end{bmatrix}^\top \begin{bmatrix} \nabla_w h \\ \nabla_q h \end{bmatrix}$$

Pseudo-stationary system:

$$\begin{pmatrix} 0 & 0 & \left(\frac{\partial h}{\partial w}\right)^\top & A^\top \\ 0 & B & \left(\frac{\partial h}{\partial q}\right)^\top & \left(\frac{\partial c}{\partial q}\right)^\top \\ \frac{\partial h}{\partial w} & \frac{\partial h}{\partial q} & 0 & 0 \\ A & \frac{\partial c}{\partial q} & 0 & 0 \end{pmatrix} \begin{pmatrix} \dot{w} \\ \dot{q} \\ \dot{\mu} \\ \dot{\lambda} \end{pmatrix} = \begin{pmatrix} -\nabla_w L \\ -\nabla_q L \\ -h \\ -c \end{pmatrix}.$$

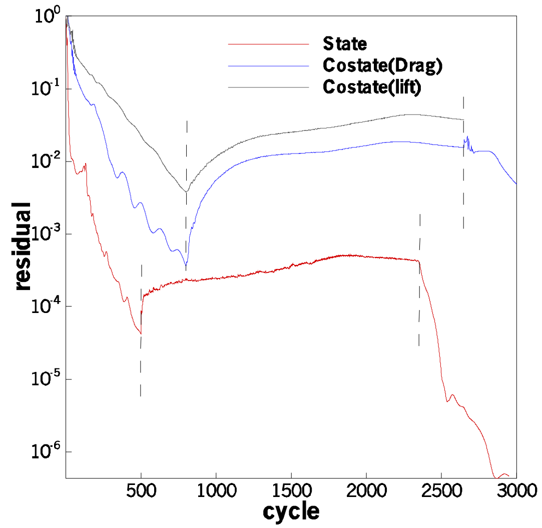
The pseudo-timestepping cycle

1) Perform 1 RK step for state equations
2) Perform 1 RK step for adjoint equations for drag
3) Perform 1 RK step for adjoint equations for lift
4) Solve the QP:

$$\min \; \frac{1}{2}\dot{q}^\top B\dot{q} + g_{lift}^\top \dot{q}$$
$$\text{s.t. } g_h^\top \dot{q} = -h(w,q) + \underline{\frac{\partial h}{\partial w}\dot{w}_{fwd}}$$

5) Perform 1 explicit Euler step for design equation

Convergence history



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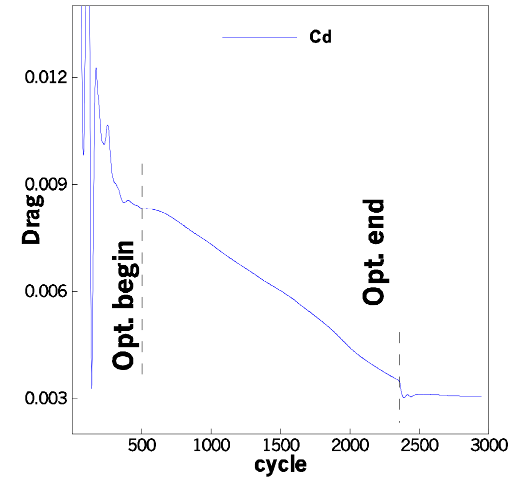

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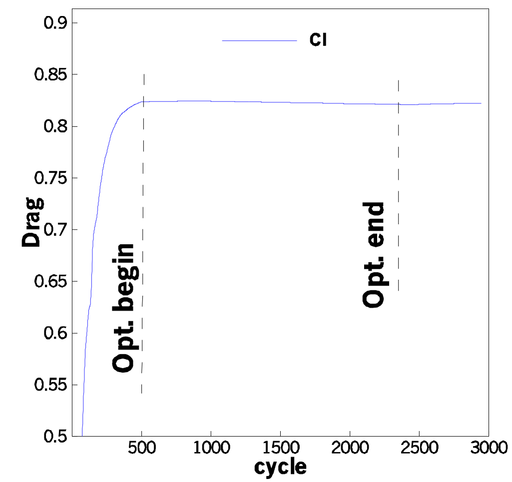

$$\Rightarrow \frac{\text{optimization effort}}{\text{state effort}} < 7$$

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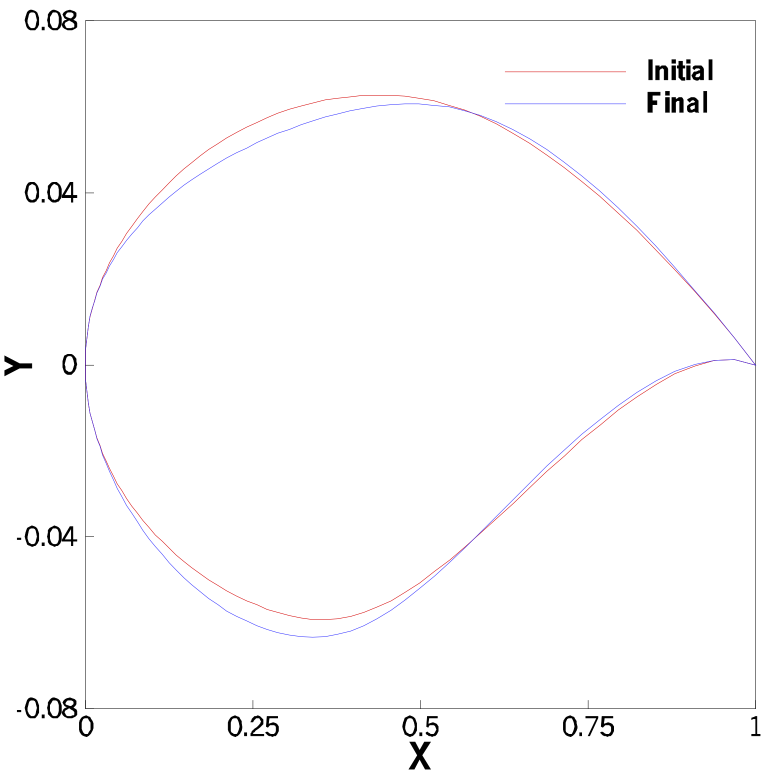
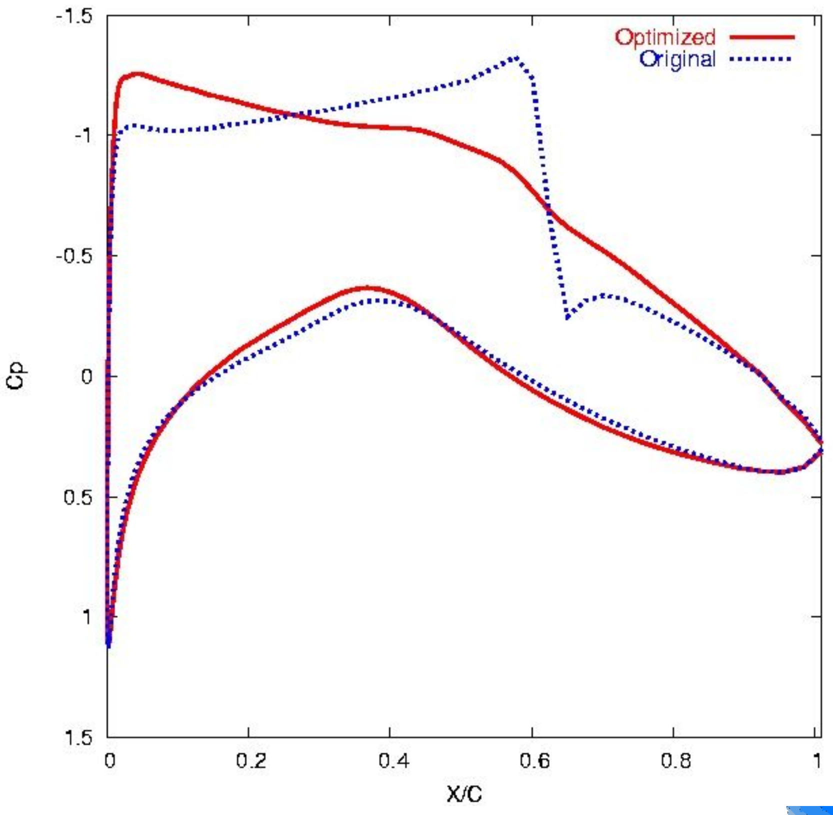
2D-results for the constrained case





Complexity measurements

- The overall cost of solving the optimization problem is roughly 4 times the cost of the forward problem (without lift constr.)

- Cost with lift constraint. = 7 times the forward problem

Lift & pitching moment constraints

minimize **drag**

s.t. **lift >= c0**

moment >= c1

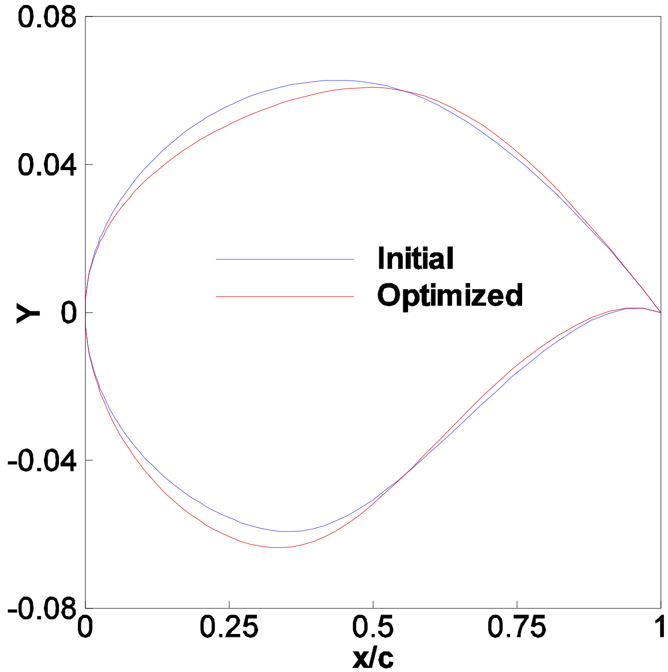
The pseudo-timestepping cycle

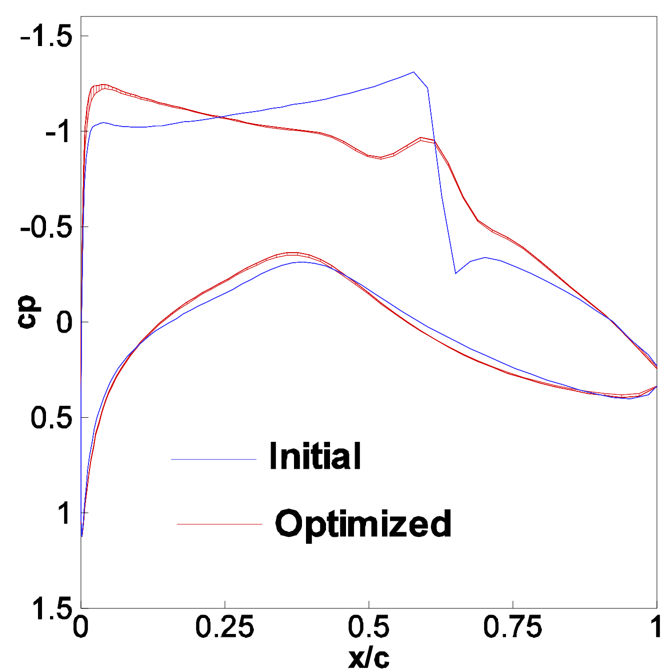
1) Perform 1 RK step for state equations
2) Perform 1 RK step for adjoint equations for drag
3) Perform 1 RK step for adjoint equations for lift
4) Perform 2 RK step for adjoint equations for moment
5) Solve the QP:

$$\min \ \frac{1}{2}\dot{q}^\top B\dot{q} + g_{\text{drag}}^\top \dot{q}$$
$$\text{s.t. } g_h^\top \dot{q} = -h(u,q) + \frac{\partial h}{\partial u}\dot{u}_{fwd}$$
$$g_m^\top \dot{q} = -m(u,q) + \frac{\partial m}{\partial u}\dot{u}_{fwd}$$

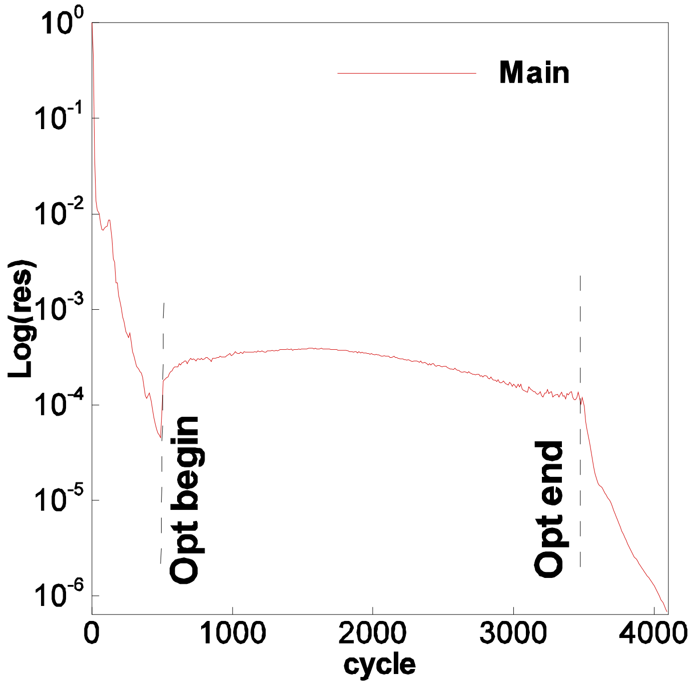
6) Perform 1 explicit Euler step for design equation

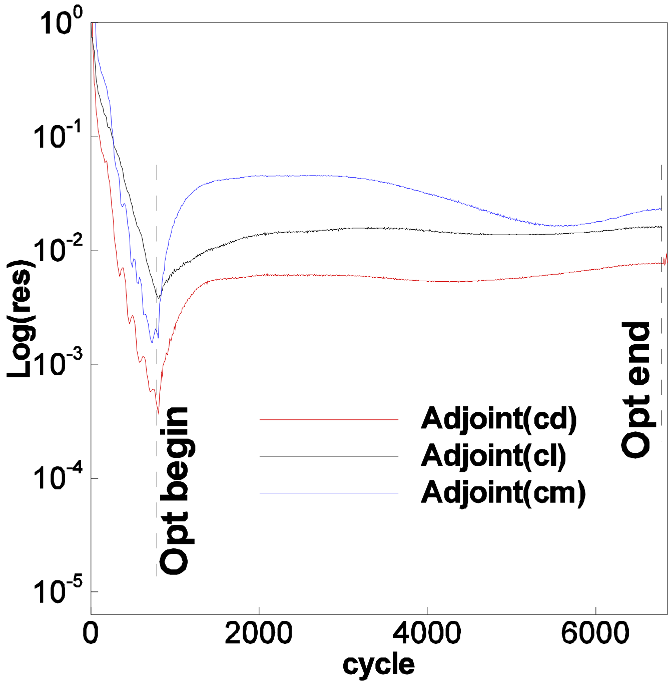
Lift & Pitching moment results





Convergence history





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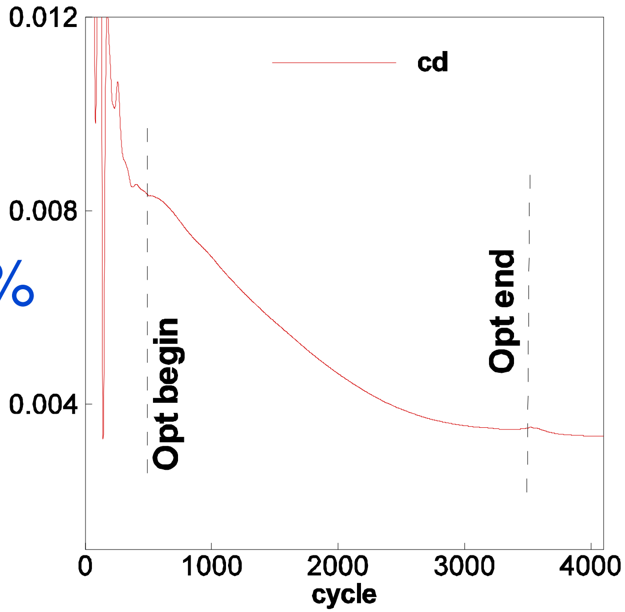
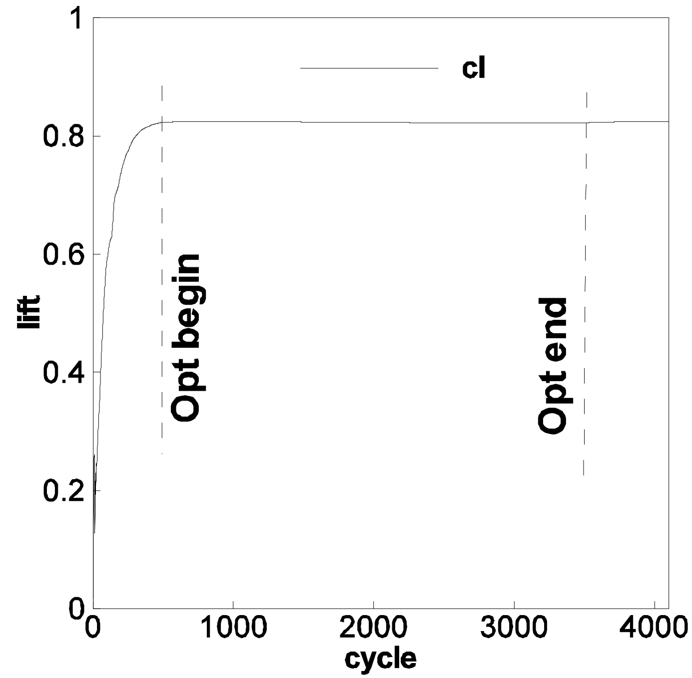
… continued

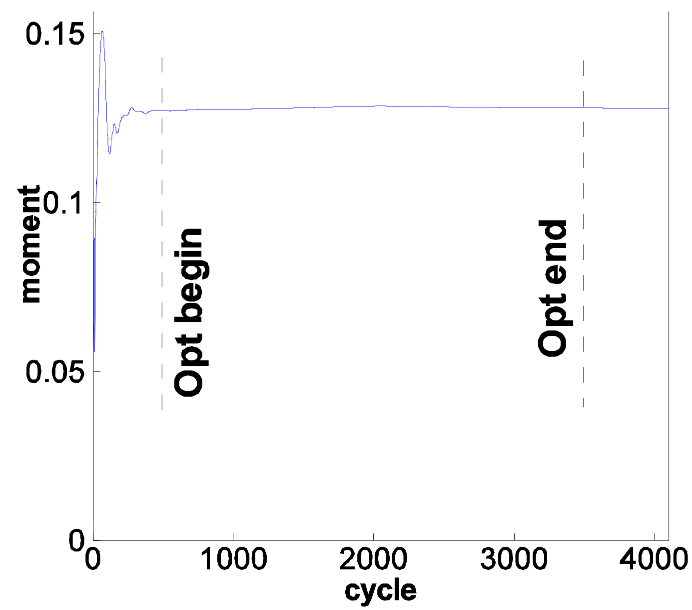
- 60%



+ 0.1%



+ 0.4%



$$\Rightarrow \frac{\text{optimization effort}}{\text{state effort}} < 10$$

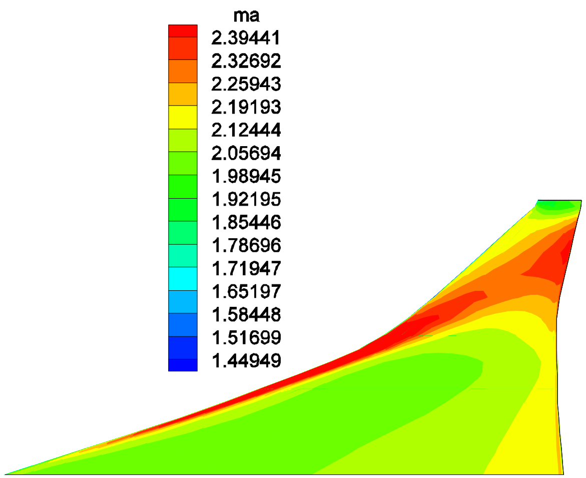
3D results for SCT wing

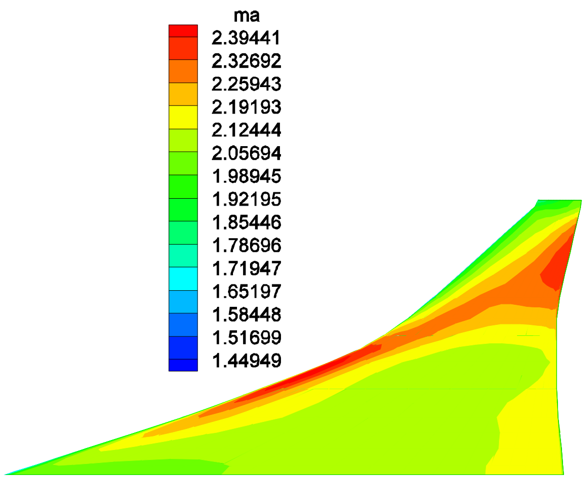
- *S*upersonic *c*ommercial *t*ransport aircraft
- Minimize drag subject to constant lift
- Drag reduced by 12.65%
- Grid: 97 x 17 x 25 = 42 225 grid nodes
- 122 geometry parameters: thickness, camberline, twist, additional DOF: angle of attack

$$\frac{\text{optimization effort}}{\text{state effort}} < 6$$

(2 initial iterations have to be spent to compute approximation of sensitivity lift versus drag)

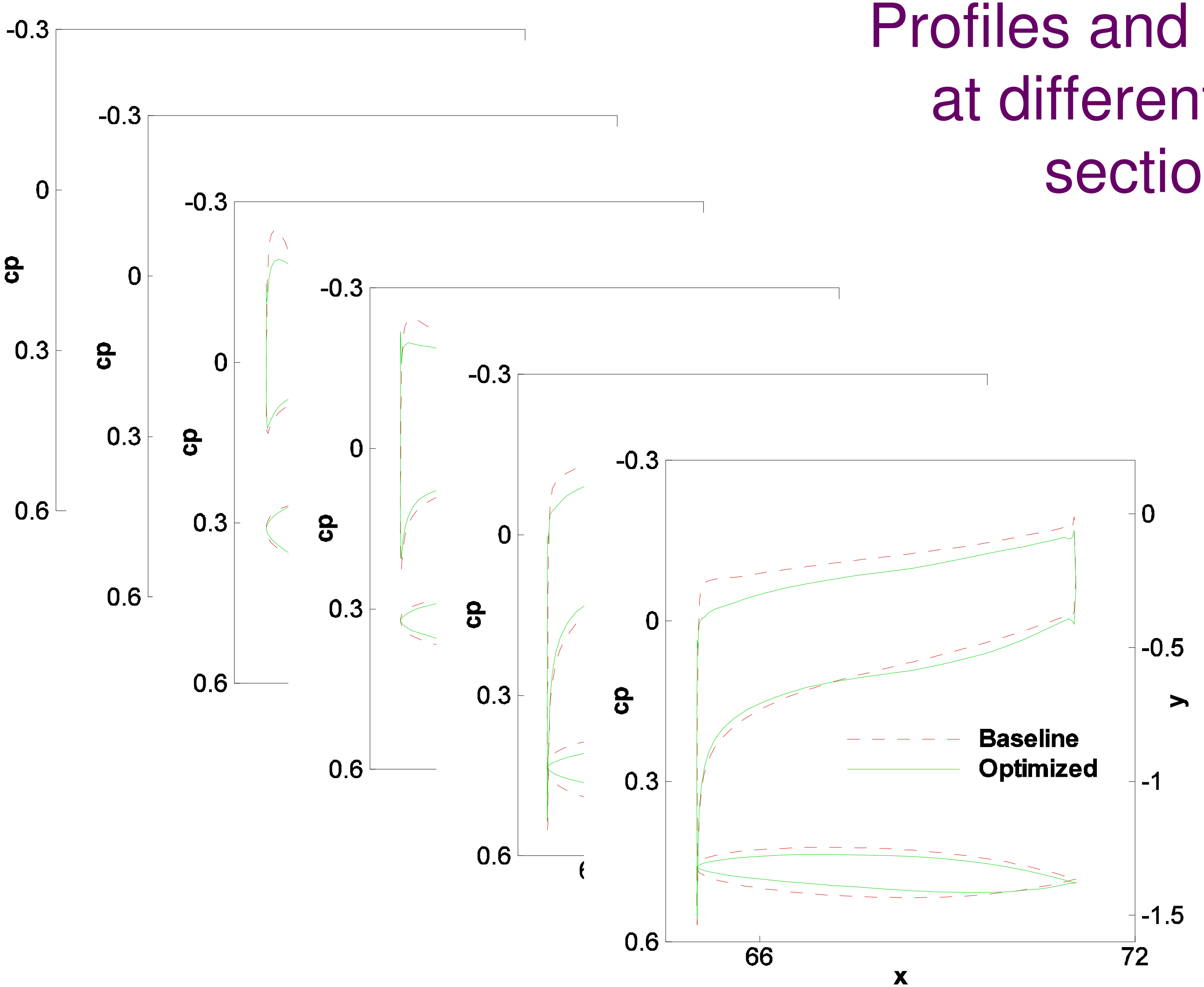
Base velocities versus optimal solution



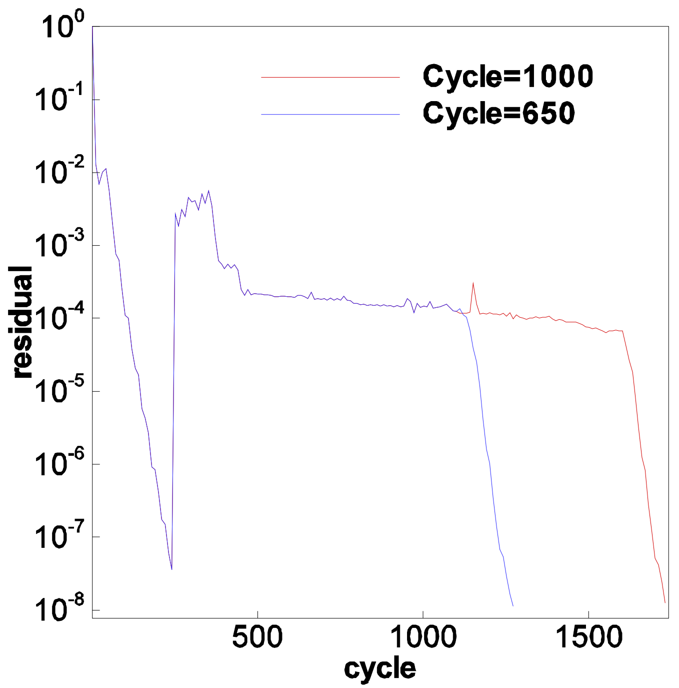


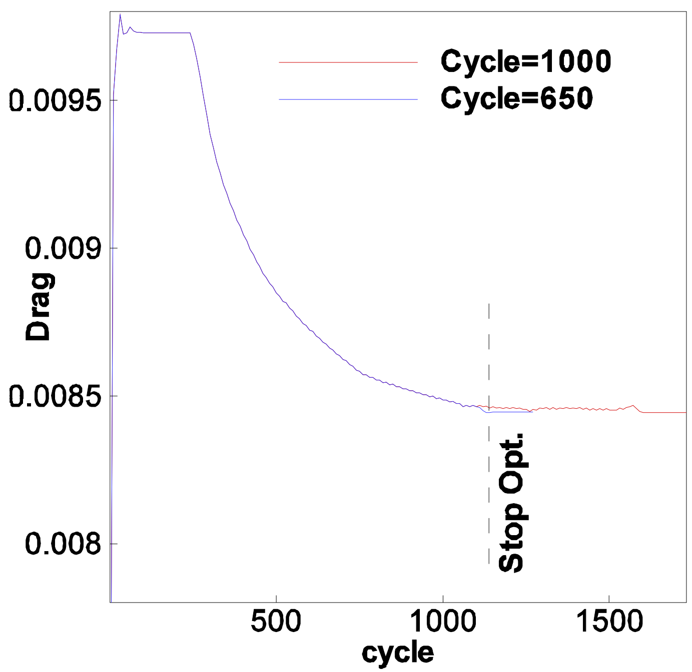
optimized

Profiles and pressure at different cross sections



Convergence history





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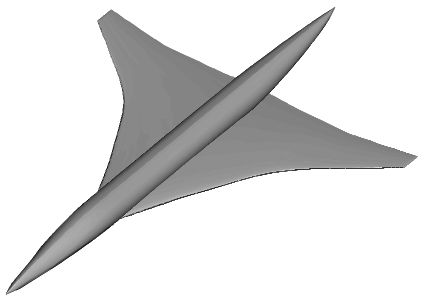
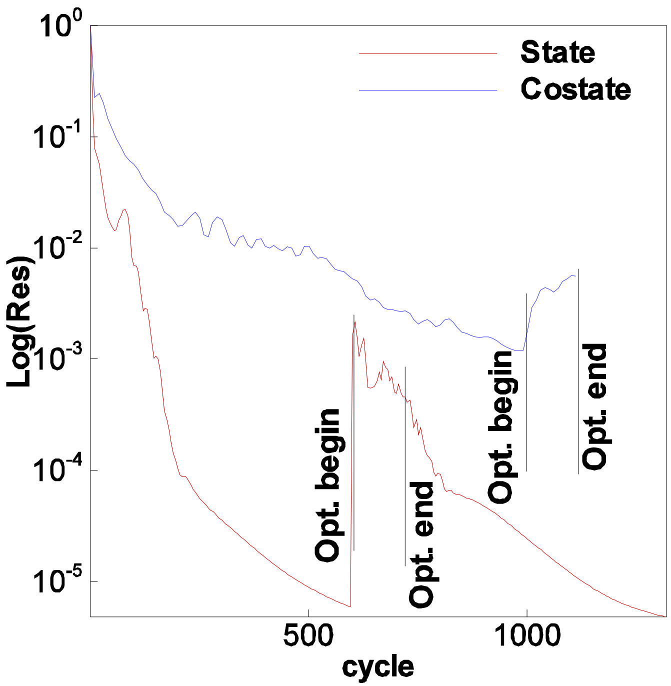
SCT body optimization

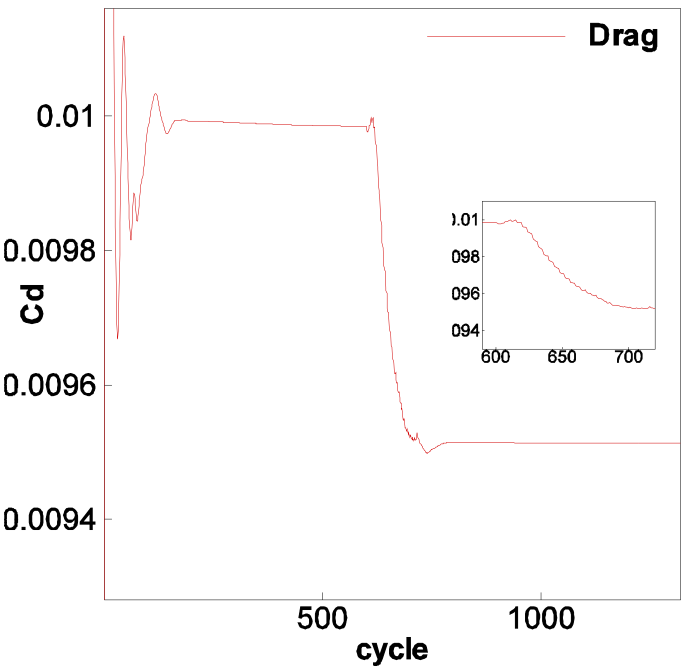


- Body only
- Minimize drag subject to constant lift
- Drag reduced by 4%
- Grid: ~ 2*10^5 grid nodes
- 10 geometry parameters: 10 radii

  additional DOF: angle of attack

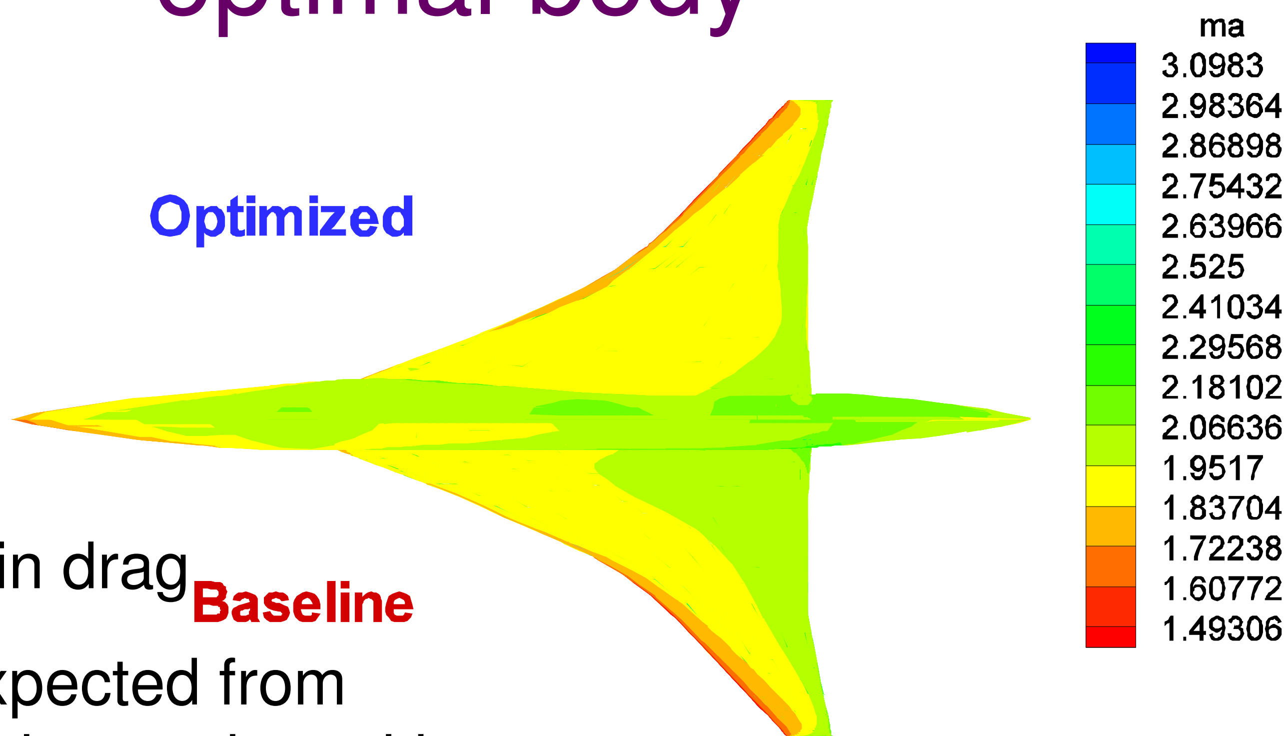
Convergence history





90 optimization cycles/ drag reduction by 4%

Combining optimal wing with optimal body



11% reduction in drag

More can be expected from optimization body together with wing

-> implementational issues…

Conclusions

- one-shot optimization based on reduced SQP ideas
- Overall computational complexity is reduced considerably.
- Limiting factor so far: frequent design space necessitate freqent calls to CAD