

One-Shot Optimization with Steady and Unsteady PDEs

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Outline

- **Consistent and Robust Discrete Adjoints**
- **Application to Separation Control on the 3D High-Lift Configuration HI-REX**
- **One-Shot Approach for Optimization with Steady PDEs**
- **Adjustments for Optimization with Unsteady PDEs**
- **One-Shot Optimization with Unsteady RANS**
- **Improving the Efficiency**
- **Numerical Results for Van der Pol Oscillator and Advection-Diffusion Equation**

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Optimality System

- **Optimization Problem:**

$$\min_{\phi \in \Phi} J(W, \phi) \quad s.t. \quad R(W, \phi) = 0$$

- **Lagrangian:**

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

- **Optimality condition (KKT system, 1. order necessary cond.):**

$$\frac{\partial L}{\partial \Lambda} = R^! = 0$$

State equation

$$\frac{\partial L}{\partial W} = \frac{\partial J}{\partial W} + \Lambda^T \frac{\partial R}{\partial W}^! = 0$$

Adjoint state equation

$$\frac{\partial L}{\partial \phi} = \frac{\partial J}{\partial \phi} + \Lambda^T \frac{\partial R}{\partial \phi}^! = 0$$

Design equation

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$$\min_{\phi \in \Phi} J(W, \phi) \quad s.t. \quad R(W, \phi) = 0$$

- **Lagrangian:** instead $L = J + \Lambda^T R$, continuous L :

$$L = J + \langle \Lambda, R \rangle_{H^*, H}$$

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$$\min_{\phi \in \Phi} J(W, \phi) \quad s.t. \quad R(W, \phi) = 0 \quad \Leftrightarrow$$

Fixed point iteration:
 $W = G(W, \phi)$

- **Lagrangian:** instead $L = J + \Lambda^T R$, continuous or discrete L :

$$L = J + \langle \Lambda, R \rangle_{H^*, H}$$

$$\Leftrightarrow L(W, \Lambda, \phi) = J(W, \phi) + \Lambda^T (G(W, \phi) - W)$$

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- Optimality condition (KKT system, 1. order necessary cond.):

Black-box differentiation:

$$\frac{\partial L}{\partial \Lambda} = G(W, \phi) - W = 0$$

State equation

$$\frac{\partial L}{\partial W} = \frac{\partial J}{\partial W} + \Lambda^T \left(\frac{\partial G}{\partial W} - I \right) = 0 \Leftrightarrow N_W^T(W, \Lambda, \phi) = \Lambda$$

Adjoint state equation

$$\frac{\partial L}{\partial \phi} = \frac{\partial J}{\partial \phi} + \Lambda^T \frac{\partial G}{\partial \phi} = 0$$

Design equation

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- Lagrangian: instead $L = J + \Lambda^T R$, continuous or discrete L :

$$L = J + \langle \Lambda, R \rangle_{H^*, H}$$

$$\Leftrightarrow L(W, \Lambda, \phi) = J(W, \phi) + \Lambda^T (G(W, \phi) - W)$$

Black-box differentiation:

$$G(W, \phi) - W = 0$$

$$\frac{\partial J}{\partial W} + \Lambda^T \left(\frac{\partial G}{\partial W} - I \right) = 0 \Leftrightarrow N_W^T(W, \Lambda, \phi) = \Lambda$$

Primal contractivity: $\|G_W\| = \|G_W^T\| \leq \rho < 1 \Rightarrow$ Adjoint contractivity:

Adjoint code inherits convergence properties of primal code

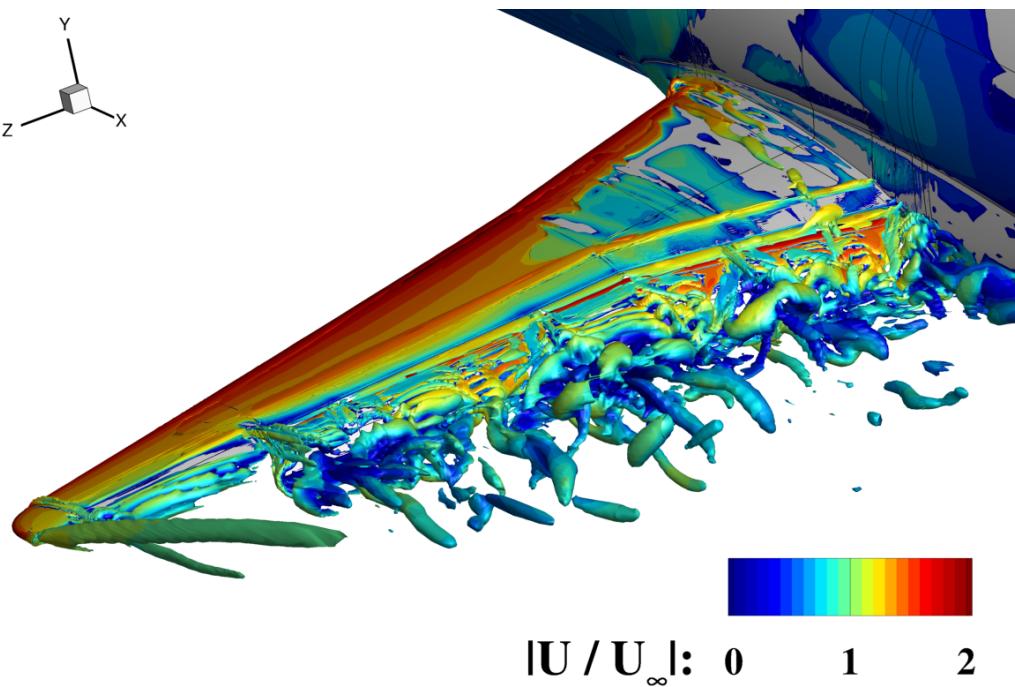
$$\left\| \frac{\partial N_W^T}{\partial \Lambda} \right\| = \|G_W^T\| \leq \rho < 1$$

Outline

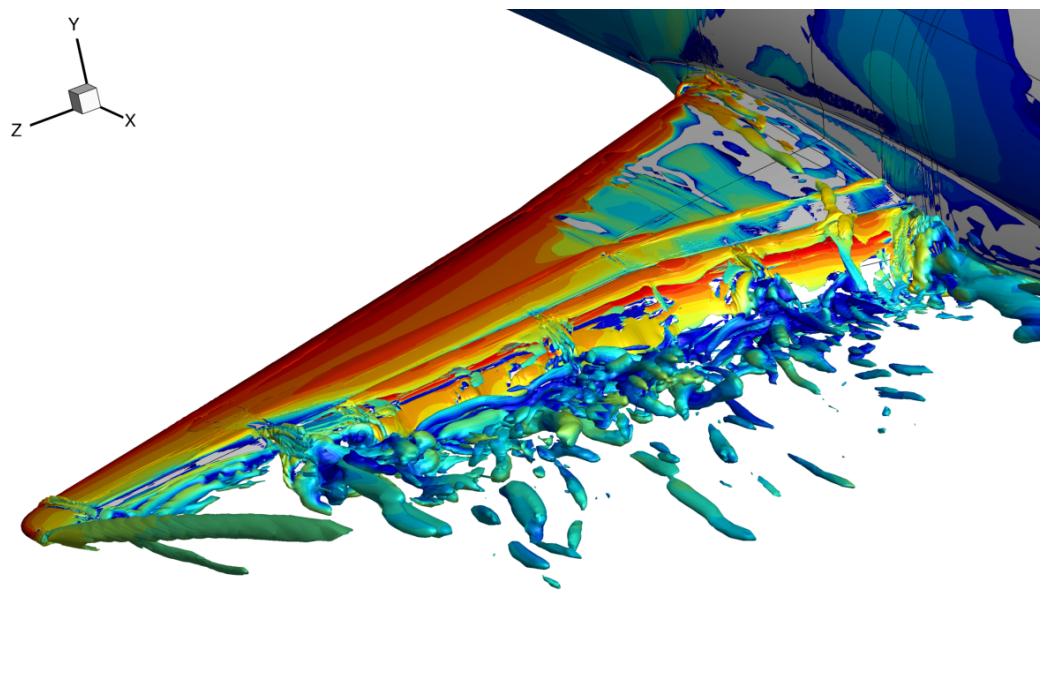
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Optimal Separation Control on Airbus HI-REX Configuration

(Primal) Flow Simulation



Un-actuated flow

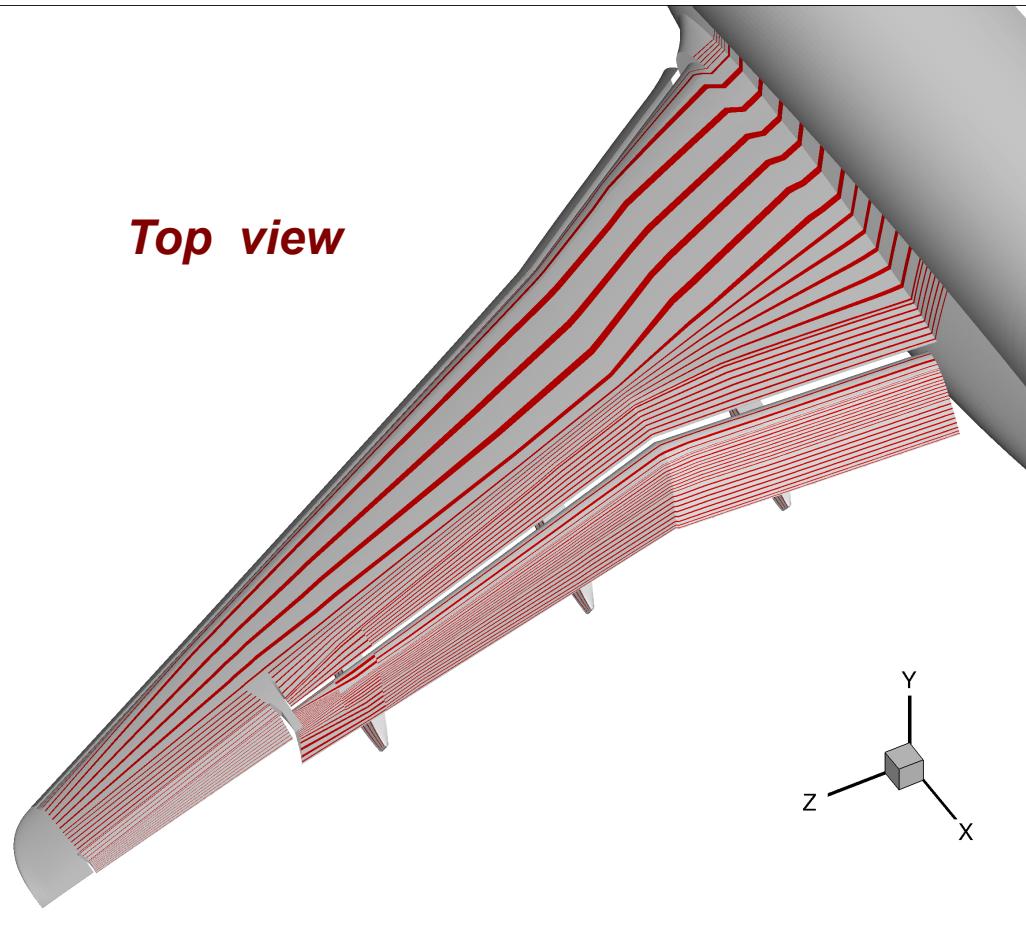


Actuated flow

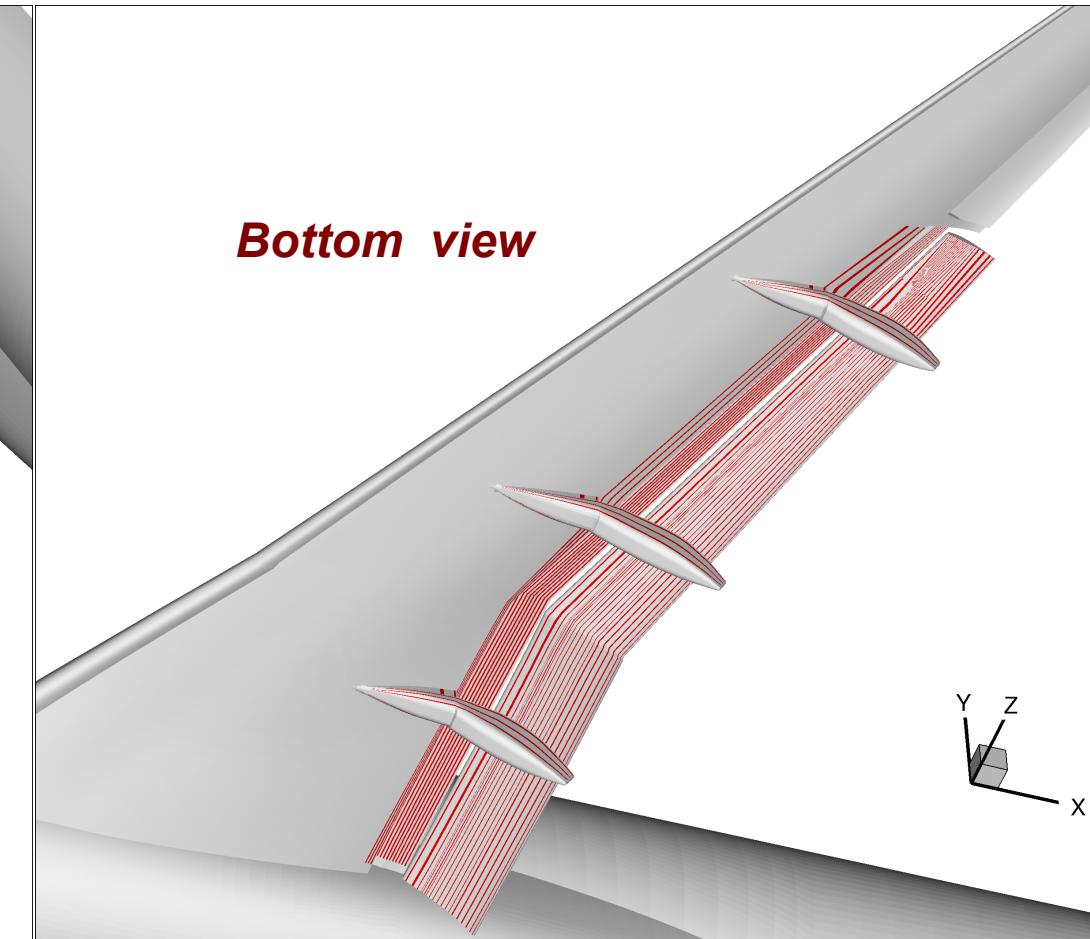
- *Grid size : 48 Million cells*
- *Re= : 1.5×10^6 , AoA= 7°*
- *ELAN Code (TU Berlin)*

Actuation slot distribution on HI-REX

Top view



Bottom view



- 33,441 synthetic jet actuators on wing and flap

Actuation boundary condition:

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix} = A \left[\vec{n} + \frac{1}{\tan \beta_1} \vec{t}_1 + \frac{1}{\tan \beta_2} \vec{t}_2 \right] \cos(2\pi f(t - t_0))$$

- No. of control variables : 167, 205

Control variables:

$$\begin{cases} A & - \text{Amplitude} \\ \beta_{1,2} & - \text{Angles} \\ t_0 & - \text{Phase shift} \\ f & - \text{Frequency} \end{cases}$$

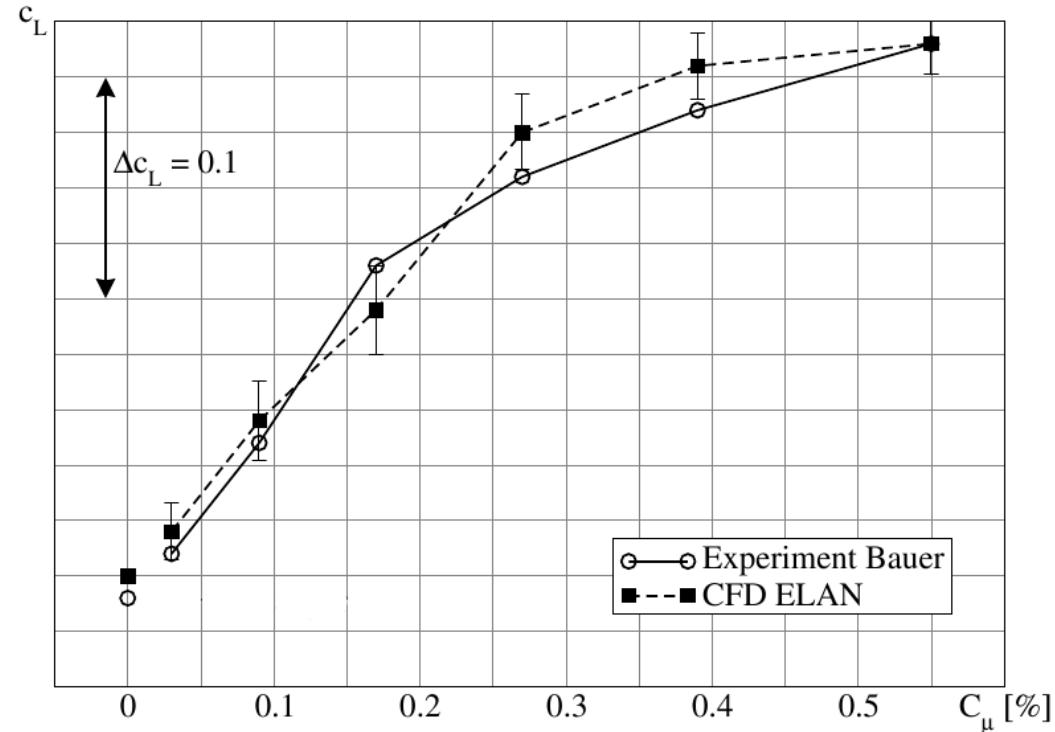
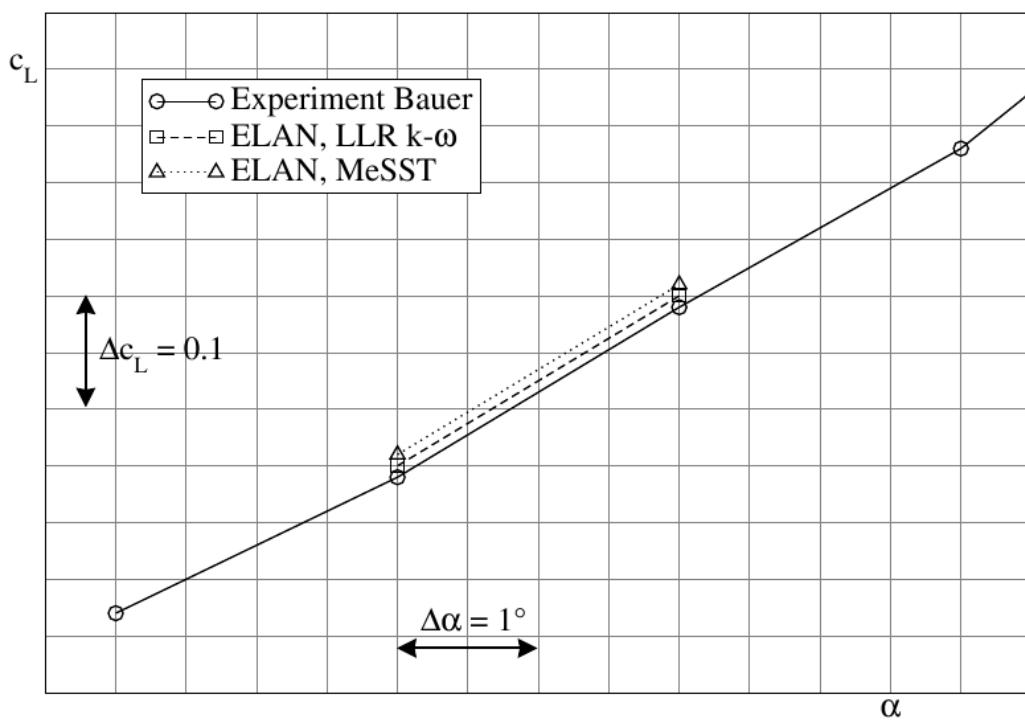
Flow Solver and Techniques for Algorithmic Differentiation

- *RANS flow solver: ELAN (TU Berlin)*
 - *Block-structured, FVM, incompressible, SIMPL*
 - *Fully implicit, MPI based parallelisation*
 - *Turbulence model : SST $k-\omega$, LLR $k-\omega$, ...*
 - *Coded in Fortran*
- *AD tool for adjoint : TAPENADE (INRIA Sophia – Antipolis)*
- *Optional: Reverse Accumulation for SIMPL loops [Christianson]*
- *Checkpointing by REVOLVE [Griewank, Walther]*
 - *Usable for Fortran and C*

Optimal Separation Control on Airbus HIREX Configuration

(Primal) Flow Simulation – Validation (Team: RWTH/TU KL, TU Berlin, Airbus)

TFB / SFB 557, DFG GA 857/5-1



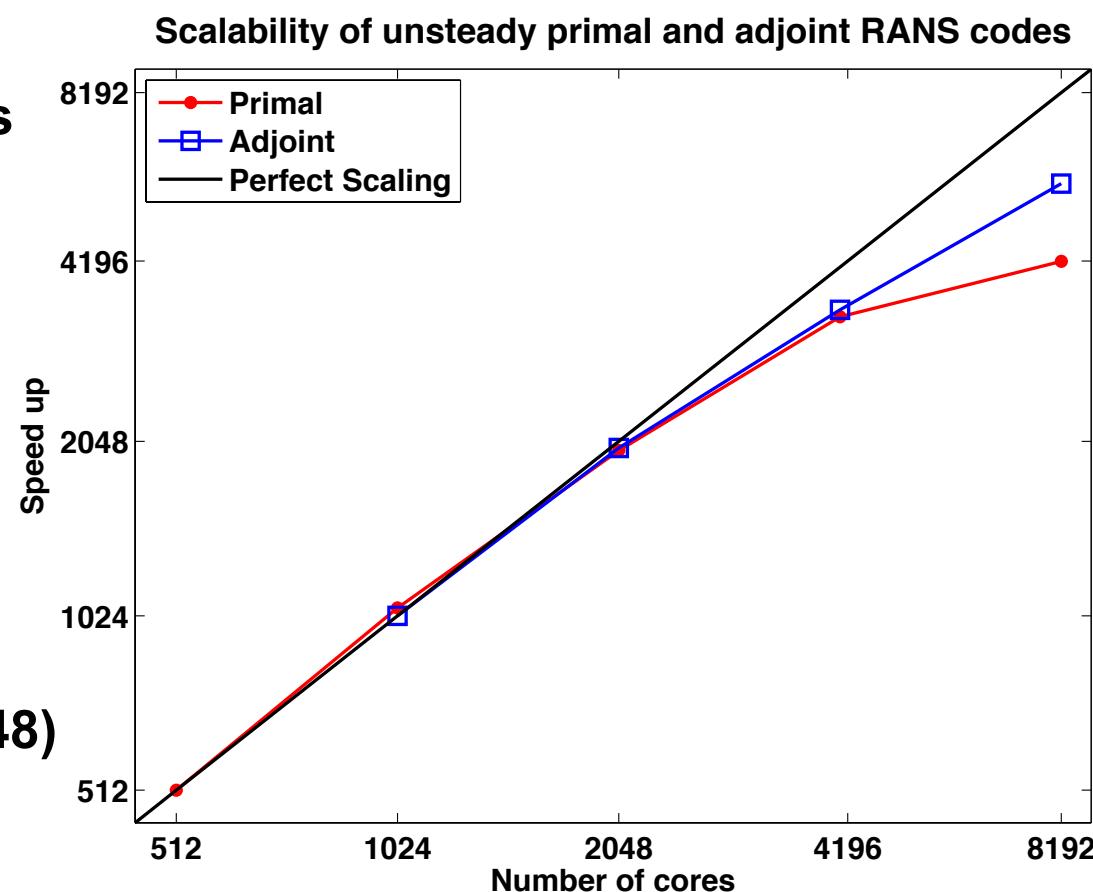
Variation of mean lift with angle of attack

- Grid size : 48 Million cells
- $Re = : 1.5 \times 10^6$, $AoA=7^\circ$

Variation of mean lift with actuation intensity

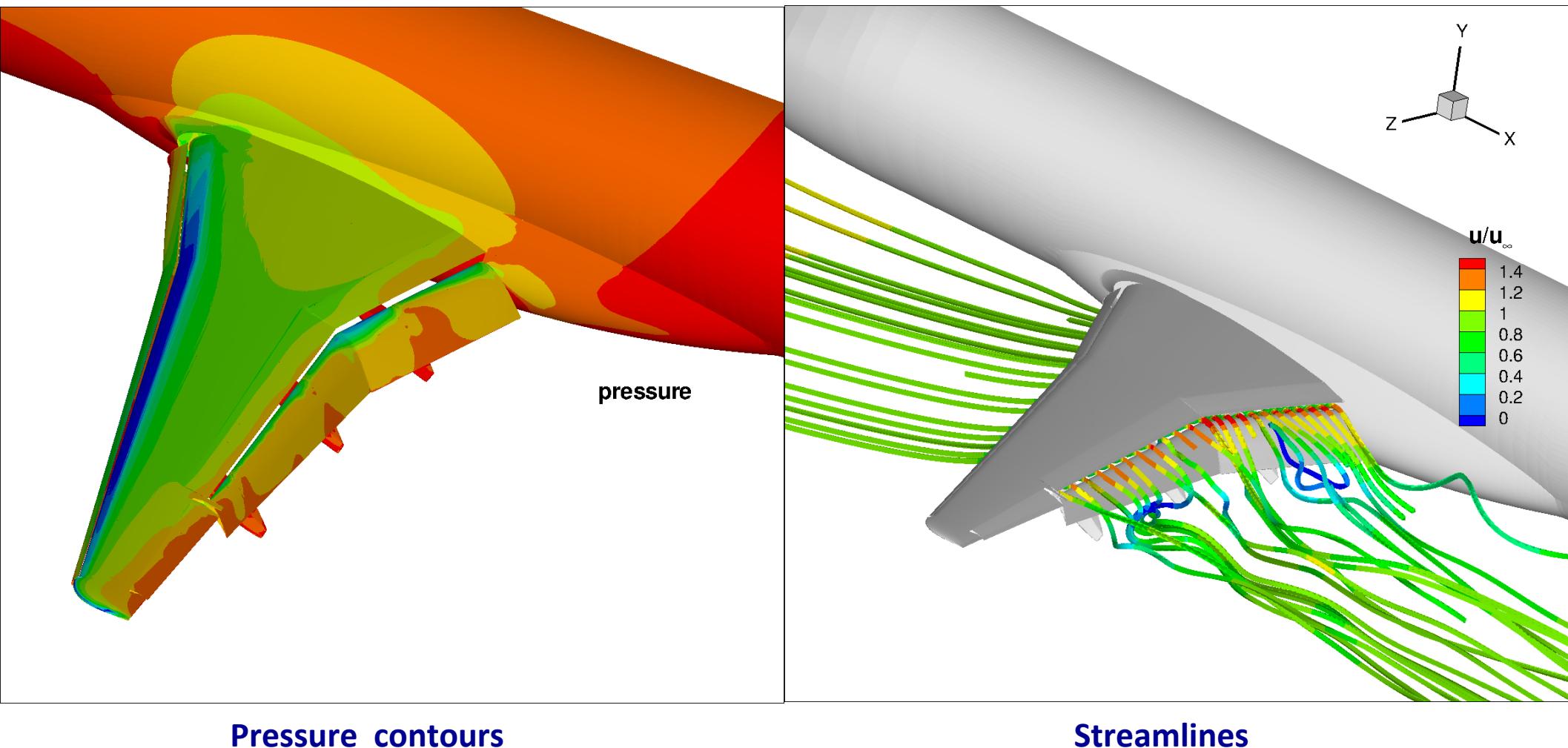
Scalability of ELAN Code (Primal / Adjoint)

- Simulations are performed on JUQUEEN (IBM Blue Gene/Q) at Jülich, Germany
- IBM PowerPC A2, 16 cores/node, 1.6 GHz, 1GB RAM/core
- Number of cores : 458,752
- Peak performance : ~6 Peta Flops
- No. of cells : 33,554,432
- No. of blocks : 8,192
- Cells/core on 8,192 cores : 4,096
- Cells/core on 512 cores : 65,536
- (Cells/core on 16,384 cores : 2,048)



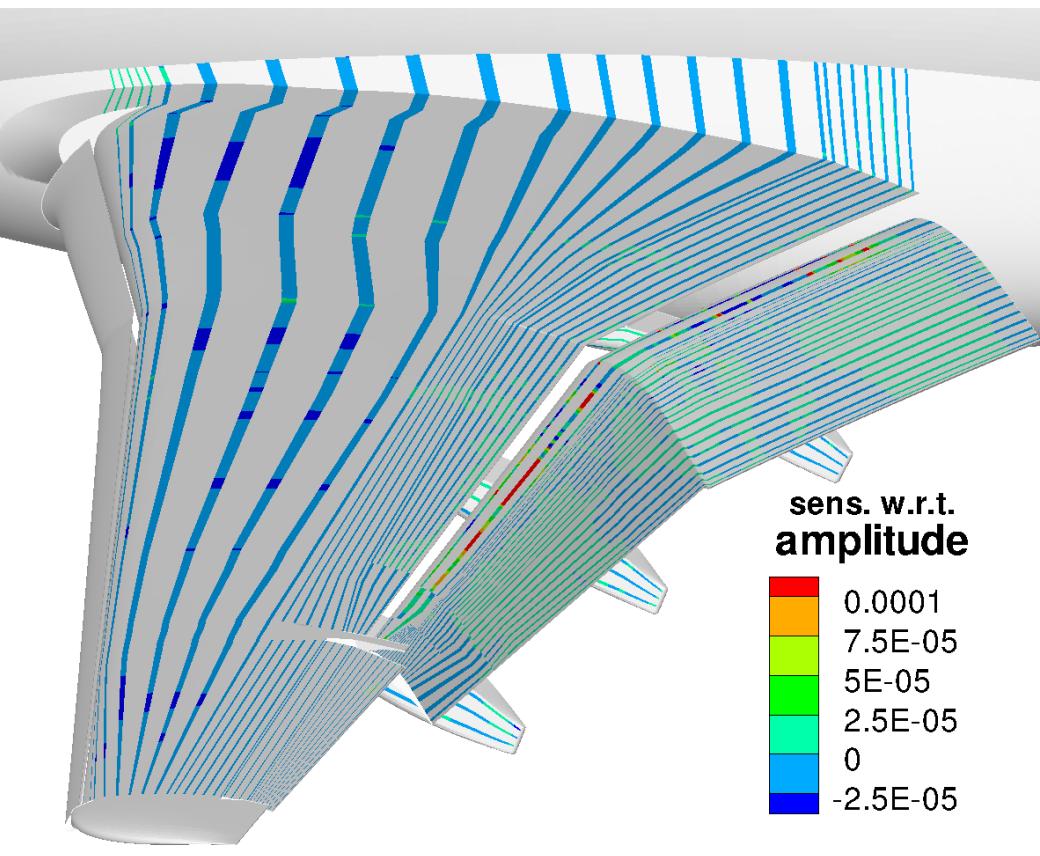
Numerical Results

Initial actuated flow: $A / u_\infty = 0.00736, f = 200Hz, t_0 = 0, \beta_{1,2} = 90^\circ$

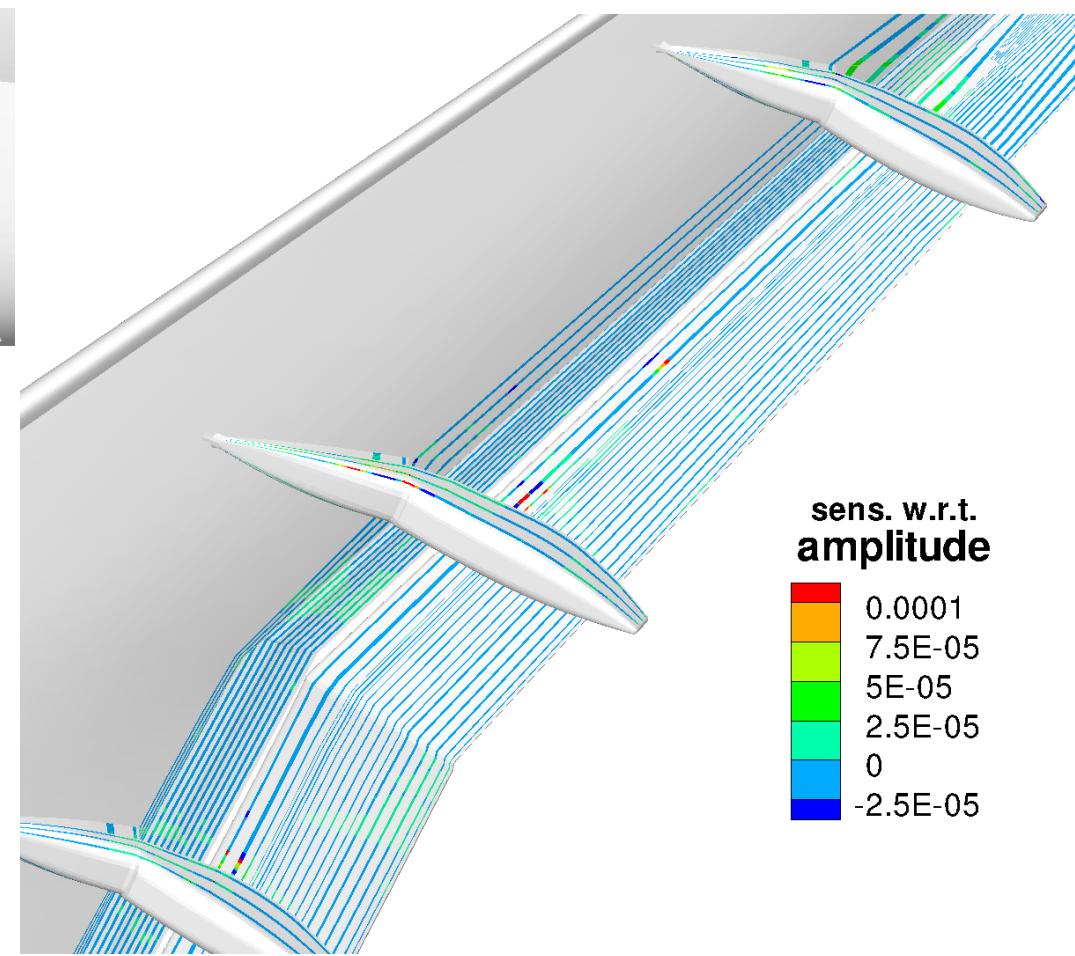


Numerical Results

Amplitude sensitivities for the initial actuated flow



Top view



Bottom view

[Nemili, Özkaya, Gauger, Kramer, Höll, Thiele, 2014]

Numerical Results

Validation of the 3D discrete adjoint URANS solver

Control parameter	Forward code	Adjoint code
Amplitude	-1.172328410564145E-05	-1.172328410564145E-05
Frequency	-2.753956866987843E-05	-2.753956866987799E-05
Phase shift	2.101437468727700E-03	2.101437468727652E-03
Blowing angle β_1	-5.469583093515221E-12	-5.469583093515383E-12
Blowing angle β_2	3.607784441402103E-12	3.607784441402158E-12

Comparison of sensitivities at a randomly selected actuation slot

[Nemili, Özkaya, Gauger, Kramer, Höll, Thiele, 2014]

Numerical Results

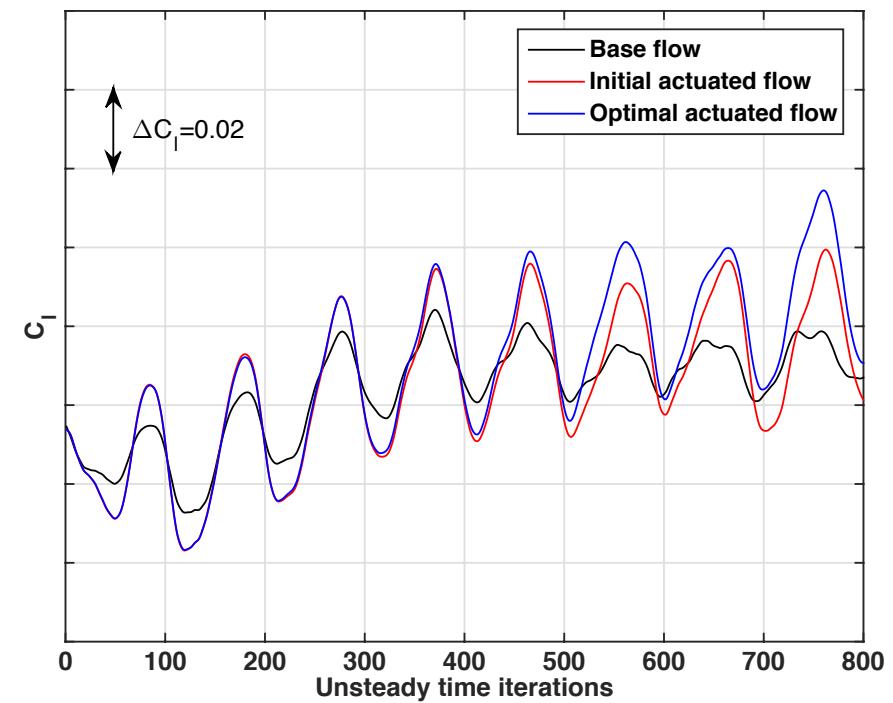
Optimal active flow control on HIREX

**Objective
function**

$$J = \bar{C}_l = \frac{1}{N - N^*} \sum_{n=N^*+1}^N C_l^n$$

$$N = 800 \text{ and } N^* = 250$$

- Optimizer: Method of steepest ascent
- Number of cycles 11
- Optimal actuation increased the mean lift by 90 counts over the base flow
by 60 counts over the initial actuation



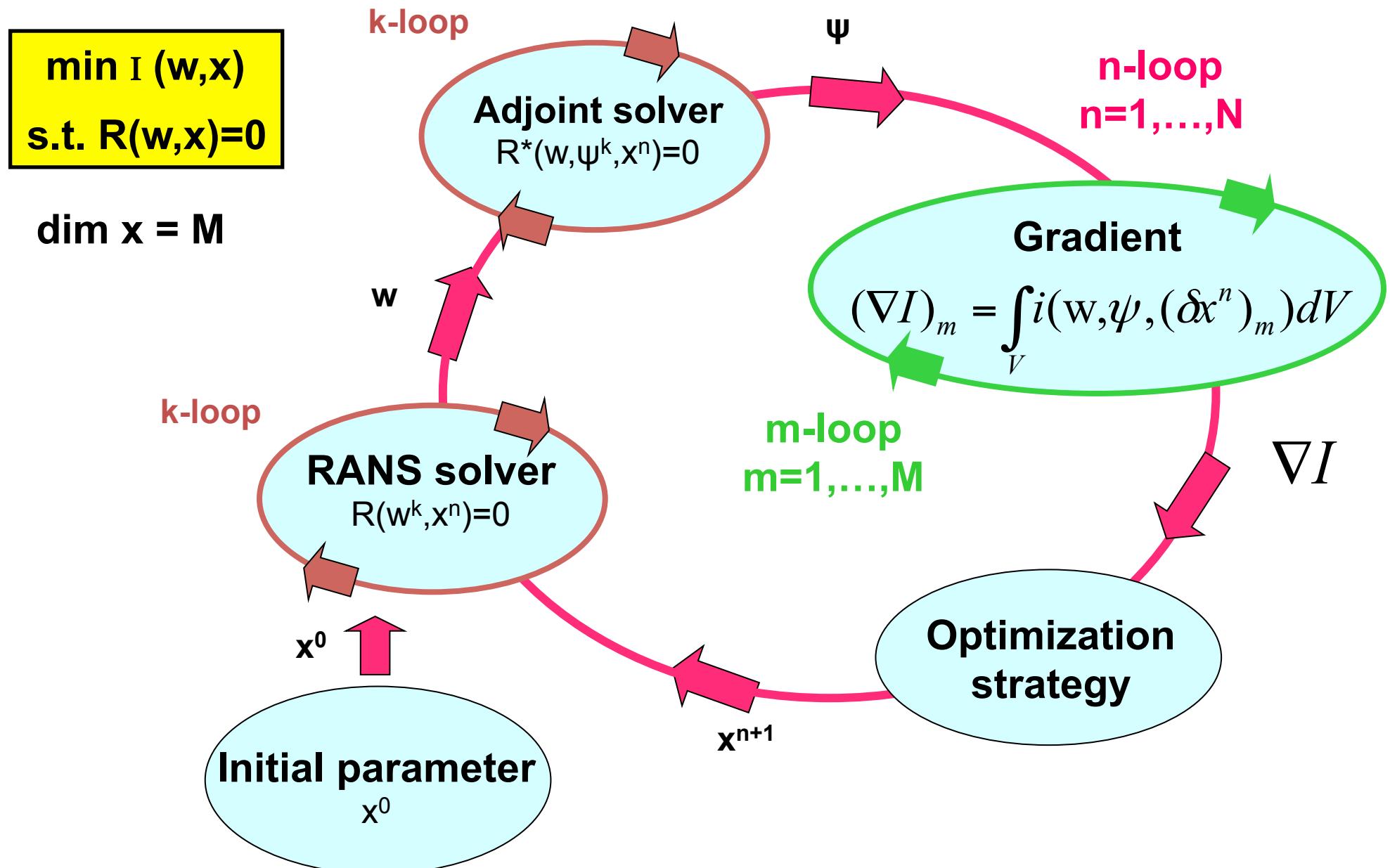
Comparison of lift for base flow,
Initial and optimal actuated flow

[Nemili, Özkaya, Gauger, Kramer, Höll, Thiele, 2014]

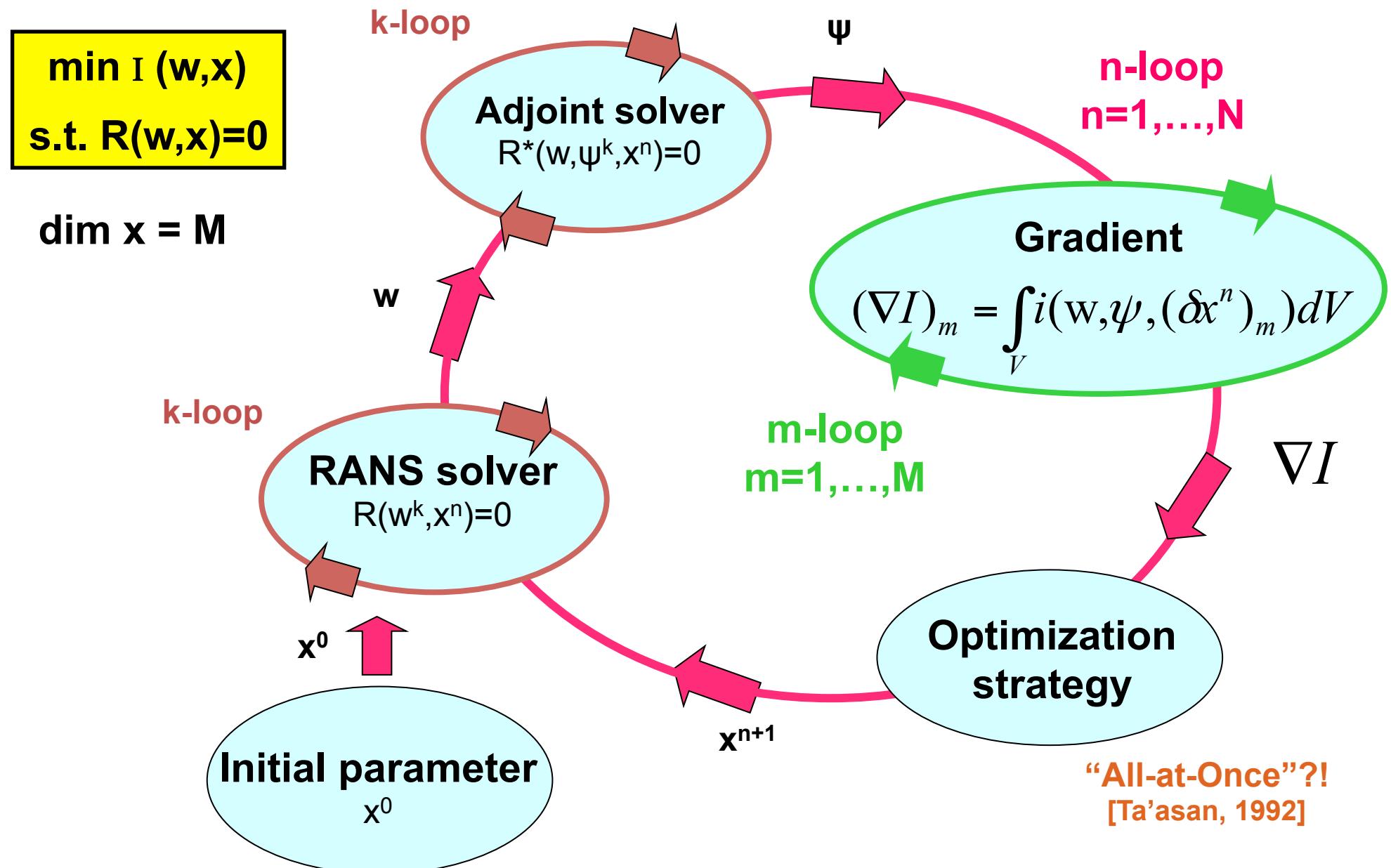
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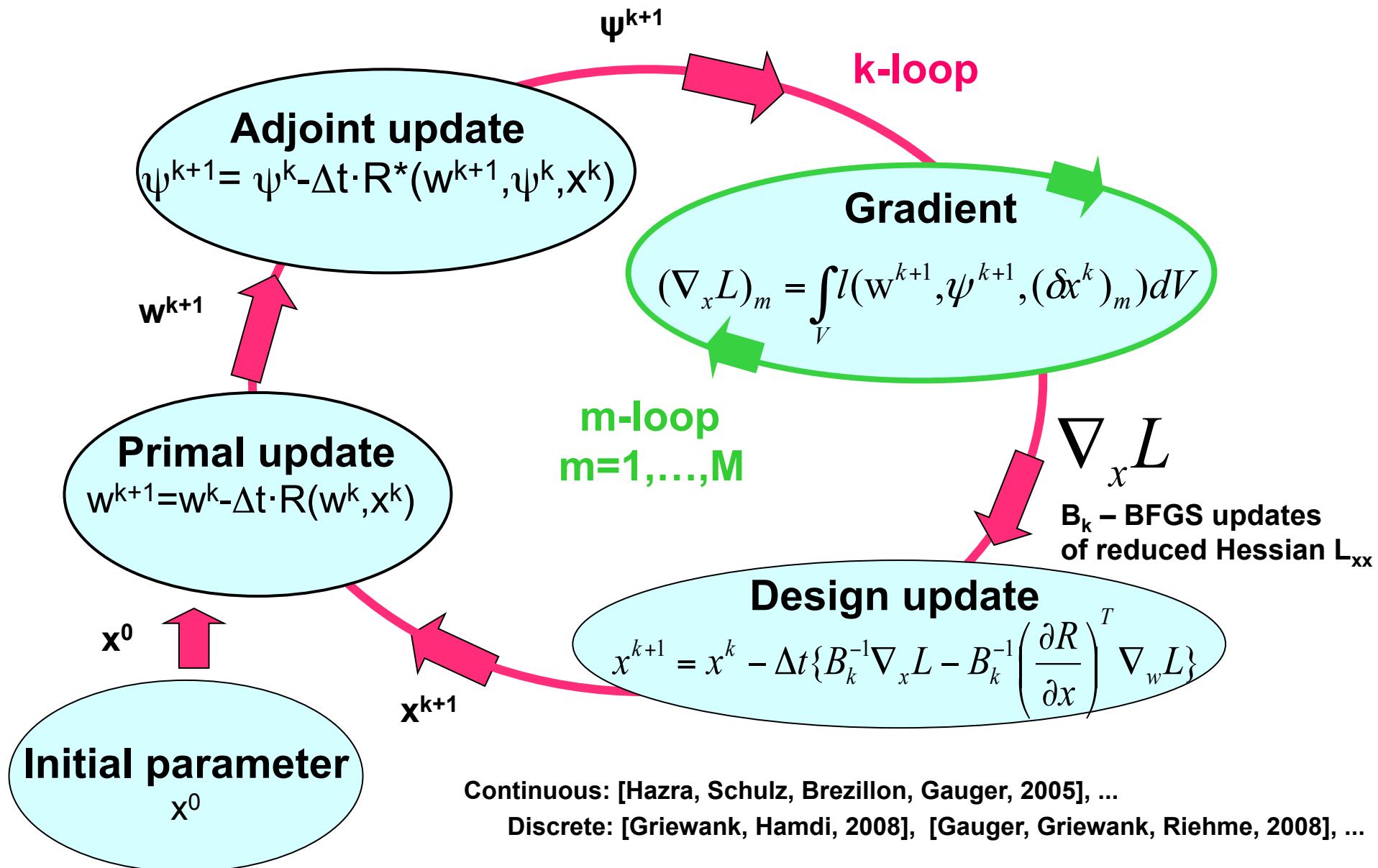
Nested Approach



Nested Approach



One-Shot Approach



Problem Setup (Steady PDE)

Goal:

$$\min_{y,u} f(y, u) \quad s.t. \quad c(y, u) = 0$$

- ▶ $y \in Y$ state variables, $u \in U$ design variables
- ▶ PDE is solved by an iterative fixed-point solver G :

$$y_{k+1} = G(y_k, u) \xrightarrow{k \rightarrow \infty} y_* = G(y_*, u)$$

Contractivity: $\left\| \frac{\partial G}{\partial y} \right\| \leq \rho < 1$

- ▶ KKT-system for $L(y, \bar{y}, u) := f(y, u) + (G(y, u) - y)^T \bar{y}$:

$$y = G(y, u)$$

State Equation

$$\bar{y} = \nabla_y f(y, u) + G_y(y, u)^T \bar{y}$$

Adjoint Equation

$$0 = \nabla_u f(y, u) + G_u(y, u)^T \bar{y}$$

Design Equation

Classical Nested vs. One-Shot Optimization Approach

► Classical nested optimization approach

Repeat for $m = 1, \dots$

- ▷ Solve for state $y_{k+1} = G(y_k, u_m) \xrightarrow{k \rightarrow \infty} y_*$
- ▷ Solve adjoint $\bar{y}_{l+1} = \nabla_y f(y_*, u_m) + G_y(y_*, u_m)^T \bar{y}_l \xrightarrow{l \rightarrow \infty} \bar{y}_*$
- ▷ Update design $u_{m+1} = u_m - B_m^{-1} (\nabla_u f(y_*, u_m) + G_u(y_*, u_m)^T \bar{y}_*)$

Classical Nested vs. One-Shot Optimization Approach

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- ▶ One-Shot optimization approach

Repeat for $k = 1, \dots$

- ▶ Update state $y_{k+1} = G(y_k, u_k)$
- ▶ Update adjoint $\bar{y}_{k+1} = \nabla_y f(y_k, u_k) + G_y(y_k, u_k)^T \bar{y}_k$
- ▶ Update design $u_{k+1} = u_k - B_k^{-1} (\nabla_u f(y_k, u_k) + G_u(y_k, u_k)^T \bar{y}_k)$

- ▶ Choice of B ensures convergence of the One-Shot method.

[Gauger, Griewank, Riehme, 2008], [Hamdi, Griewank, 2008], ...

One-Shot Approach

$$\begin{aligned} L(y, \bar{y}, u) &= f(y, u) + (G(y, u) - y)^T \bar{y} \\ &= \underbrace{N(y, \bar{y}, u)}_{\text{shifted Lagrangian}} - y^T \bar{y} \end{aligned}$$

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):

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

One-Shot Approach

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

shifted Lagrangian

Stationary point:

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

Piggy-Back

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

[Griewank,Faure 2002]

One-Shot Approach

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

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

Aims: Choose B such that:

- **Convergence of (OS)**
- **Bounded retardation**
i.e. $O(\text{opt}) / O(\text{sim}) < \text{const}$

Jacobian:

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

Doubly Augmented Lagrangian

- 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**

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

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

- Gradient of L^a :

$$\begin{bmatrix} \nabla_y L^a \\ \nabla_{\bar{y}} L^a \\ \nabla_u L^a \end{bmatrix} = - \underbrace{\begin{bmatrix} \alpha(I - G_y)^T & -I - \beta N_{yy} & 0 \\ -I & \beta(I - G_y) & 0 \\ -\alpha G_u^T & -\beta N_{yu}^T & B \end{bmatrix}}_{=: M} \underbrace{\begin{bmatrix} G(y, u) - y \\ N_y(y, \bar{y}, u)^T - \bar{y} \\ -B^{-1} N_u(y, \bar{y}, u)^T \end{bmatrix}}_{=: s}$$

one-shot increment

Descent Direction for L^a

Theorem (Correspondence condition):

L^a is an exact penalty function, if $\alpha\beta(I - G_y)^T(I - G_y) \succ I + \beta N_{yy}$.

Theorem (Descent condition):

The One-Shot increment vector $s(y, \bar{y}, u) := \begin{bmatrix} G(y, u) - y \\ N_y(y, \bar{y}, u)^T - \bar{y} \\ -B^{-1}N_u(y, \bar{y}, u)^T \end{bmatrix}$

is a descent direction for all large positive B if and only if

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

➤ Both conditions are implied by $\sqrt{\alpha\beta}(1 - \rho) > 1 + \frac{\beta}{2}\|N_{yy}\|$.

[Hamdi, Griewank, 2008], ...

[Gauger, Griewank, Hamdi, Kratzenstein, Özkaya, Slawig, 2012]

Convergence of One-Shot

- Choose $\beta = \frac{2}{c}$, $\alpha = \frac{2c}{(1-\rho)^2}$ with $c = \|N_{yy}\|$
- Choose B such that

$$B \geq B_0 := \alpha G_u^T G_u + \beta N_{yu}^T N_{yu} + N_{uu}.$$

then s yields descent on L^a .

⇒ Convergence of One-Shot approach.

[Hamdi, Griewank, 2008], ...

[Gauger, Griewank, Hamdi, Kratzenstein, Öz kaya, Slawig, 2012]

In practice: BFGS-updates for the Hessian

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

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).

[Özkaya, Gauger, 2008]

Efficient One-Shot Approach

ONERA M6, $M=0.83$, $\alpha=3.01^\circ$

Drag reduction by constant lift

DLR TAU Code (Euler)

Initial geometry:

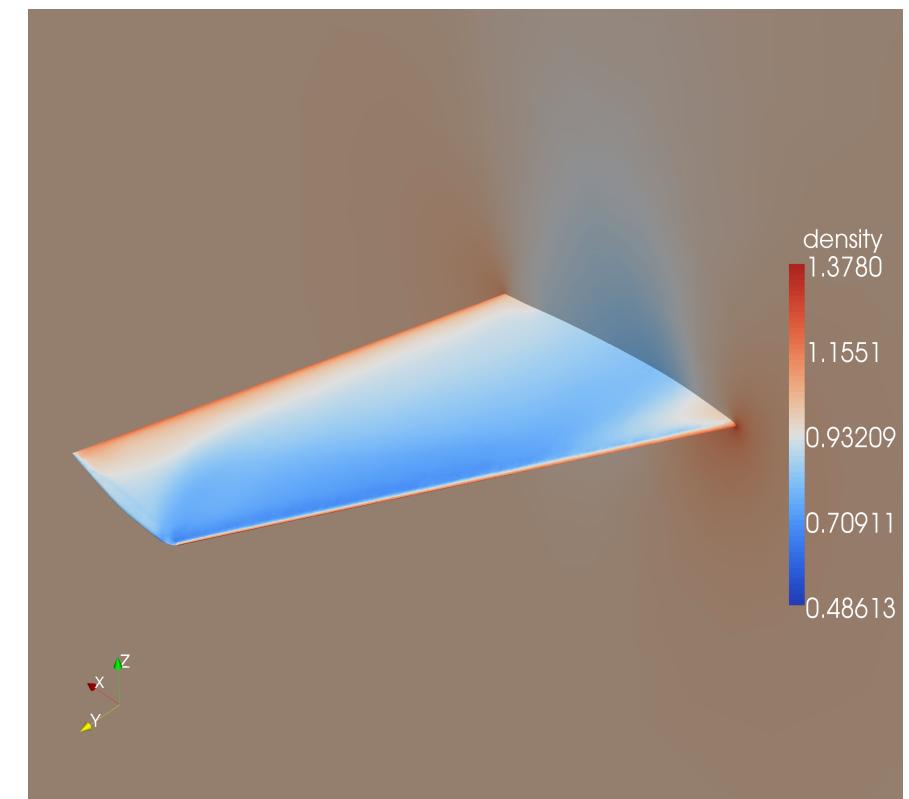
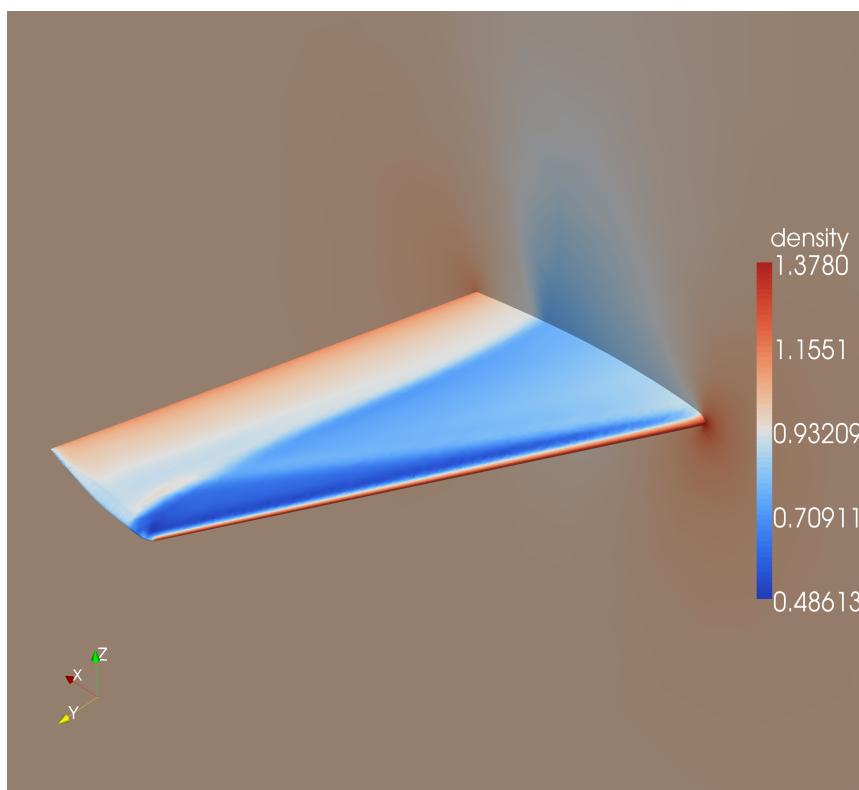
- ↗ $C_D^{\text{init}} = 106$ drag counts
- ↗ $C_L^{\text{init}} = 27.6$ lift counts

Optimized geometry:

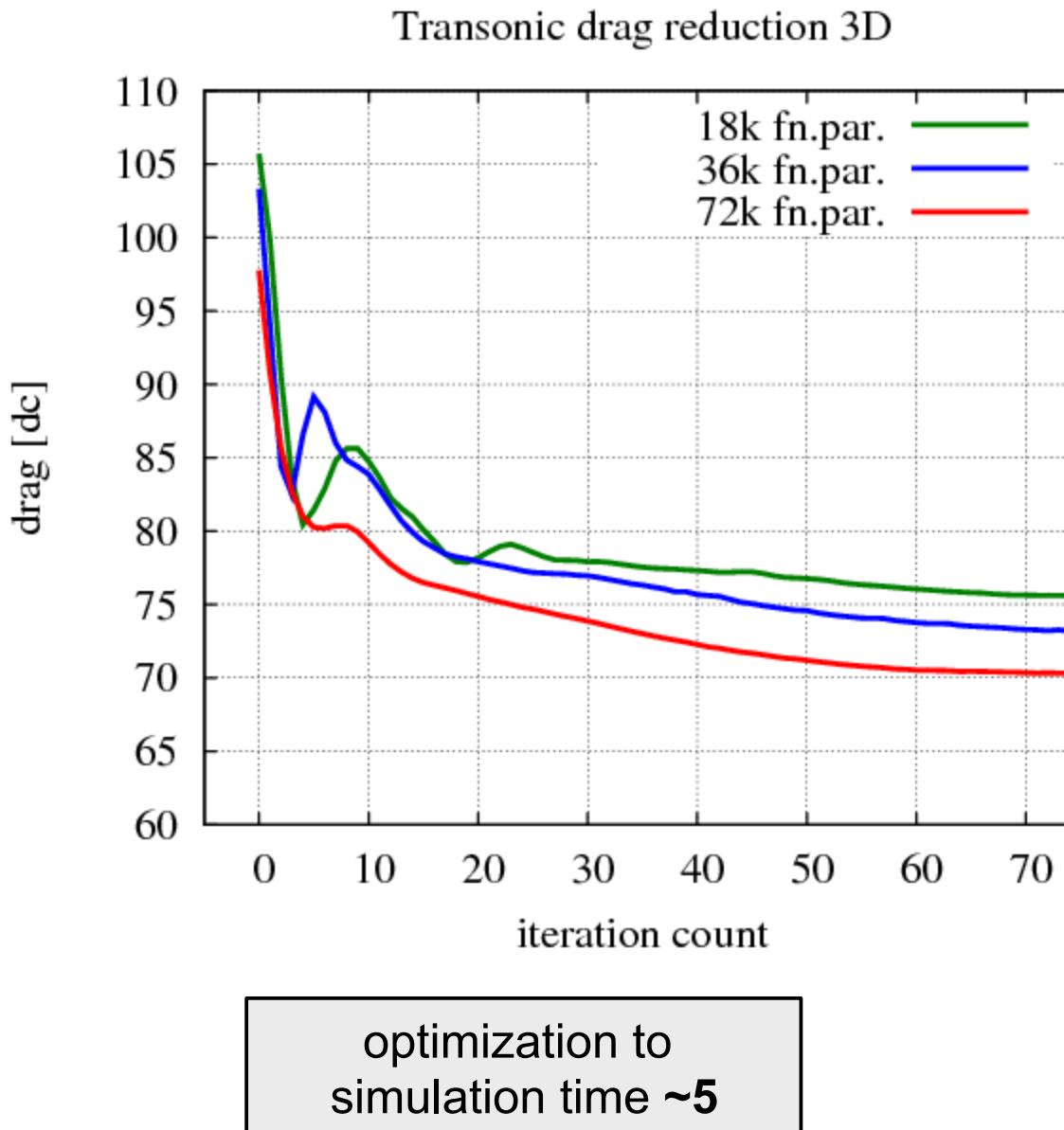
- ↗ $C_D^{\text{opt}} = 72$ drag counts
- ↗ $C_L^{\text{opt}} = 26.5$ lift counts

**O(opt) / O(sim) = 5 (wall clock time)
= 2 (# iterations)**

32% drag reduction



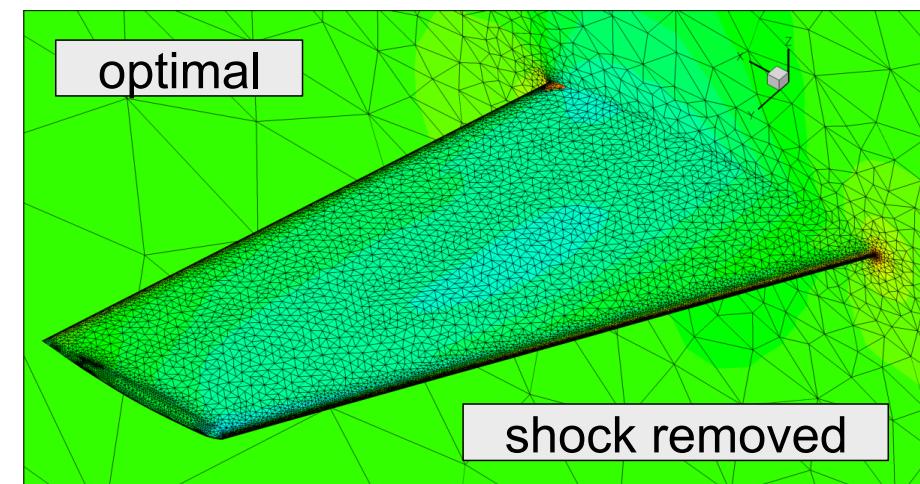
Scaling with Number of Parameters



Approach:

- ↗ Shape Derivatives
- ↗ Gradient Smoothing
- ↗ Preconditioning
- ↗ One Shot

optimal drag =
 induced drag (planform)
 + spurious drag (numerics)

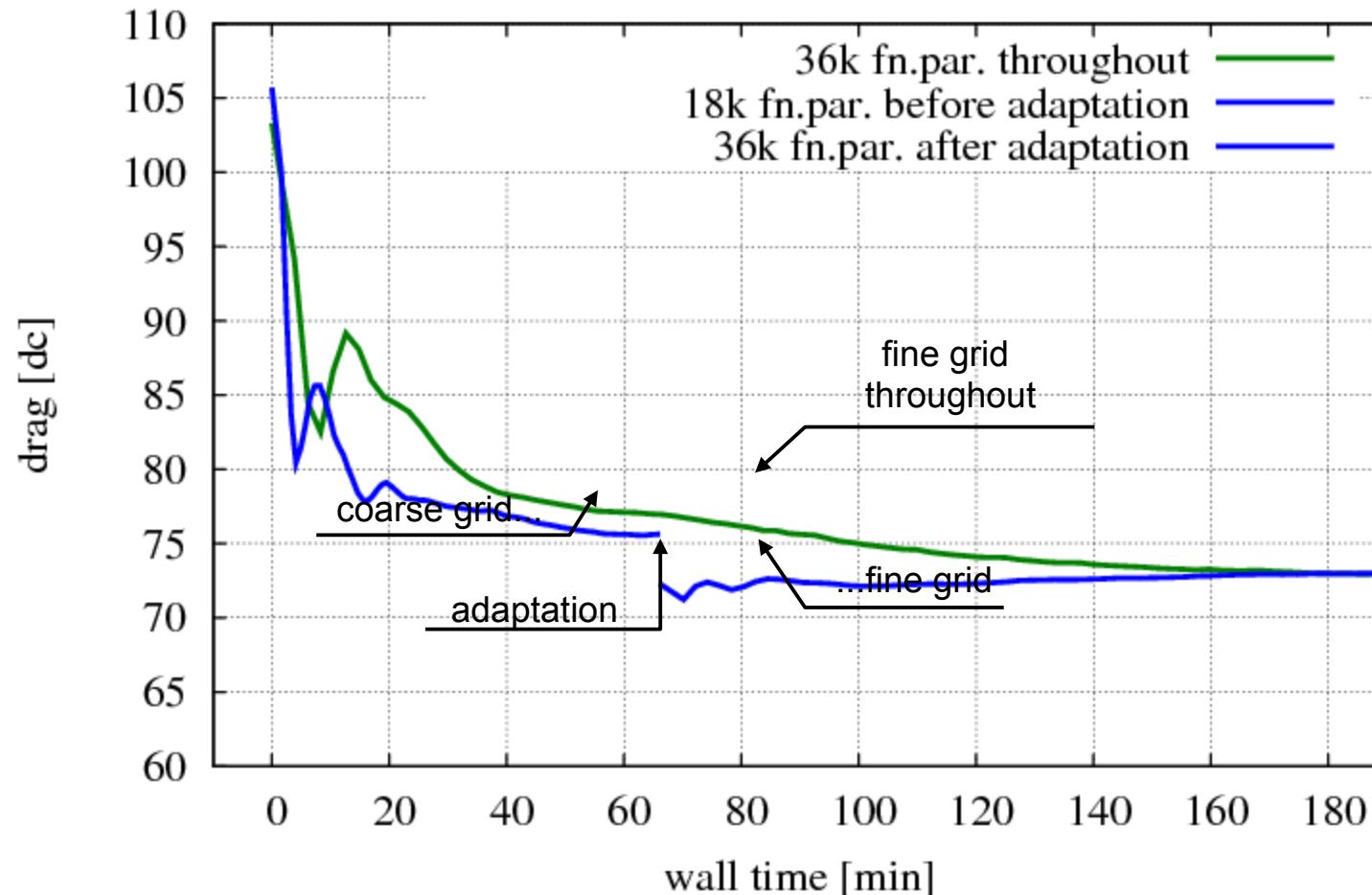


[Illic, Gauger, Schmidt, Schulz, 2009]

Multilevel Descent

➤ 2-level: coarse grid **18k** design parameters, fine **36k**

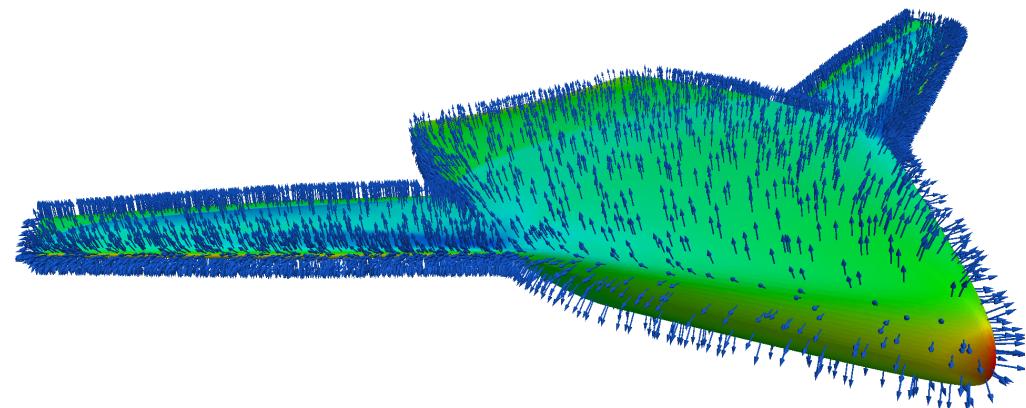
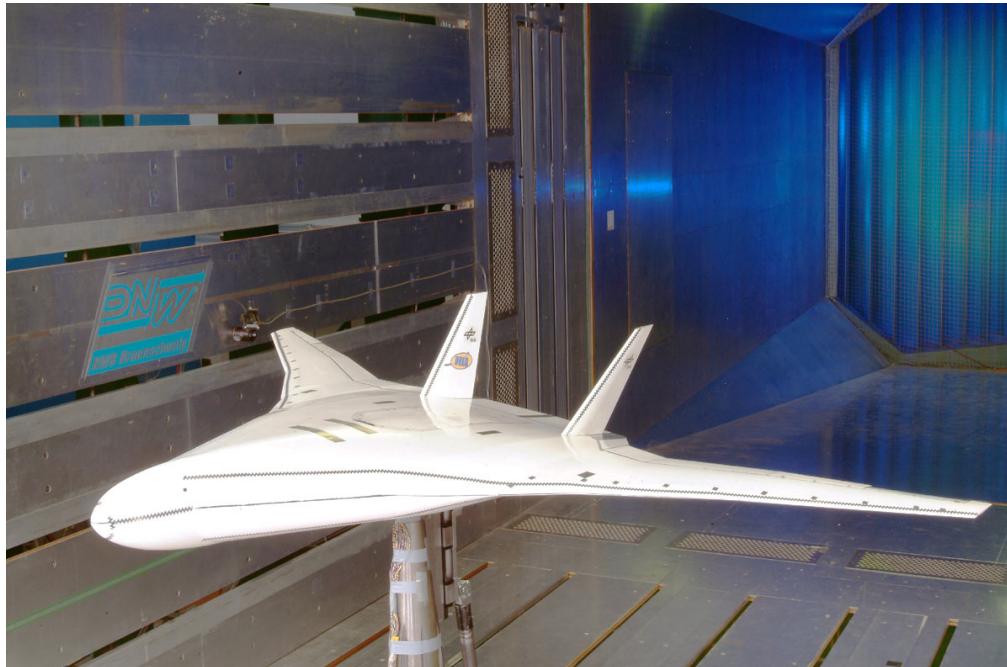
Transonic drag reduction, 3D multilevel



➤ 2-level iteration brings factor ~ 2 in optimization time

[Illic, Gauger, Schmidt, Schulz, 2009]

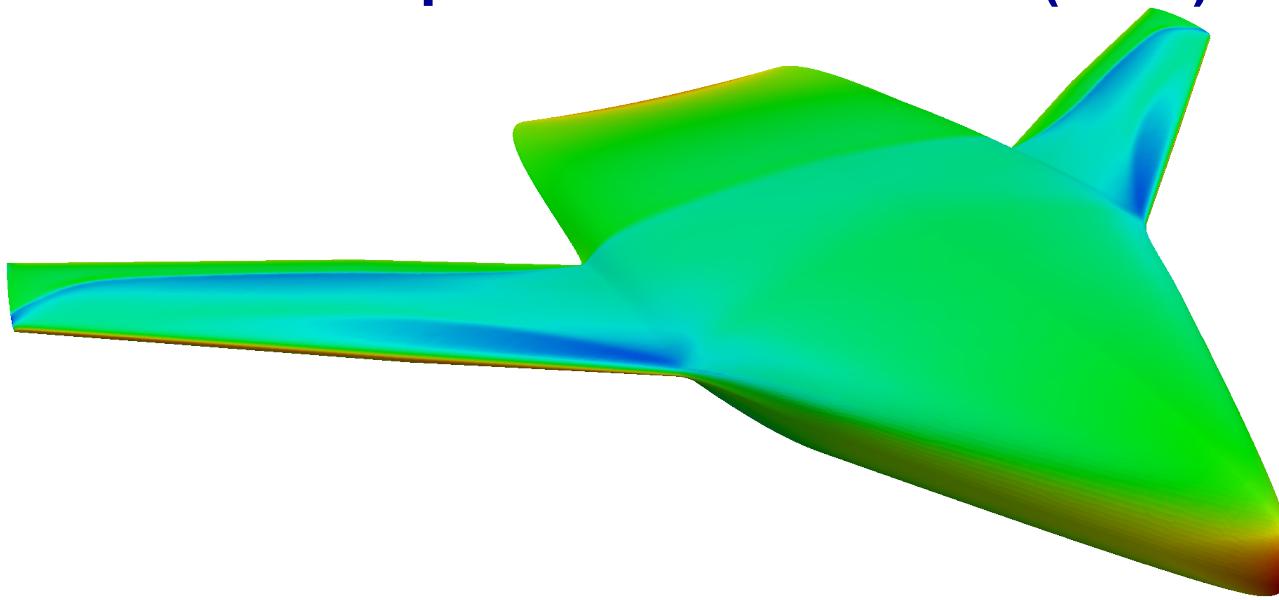
One-Shot Optimization of VELA (DLR)



Design study for blended wing-body configurations

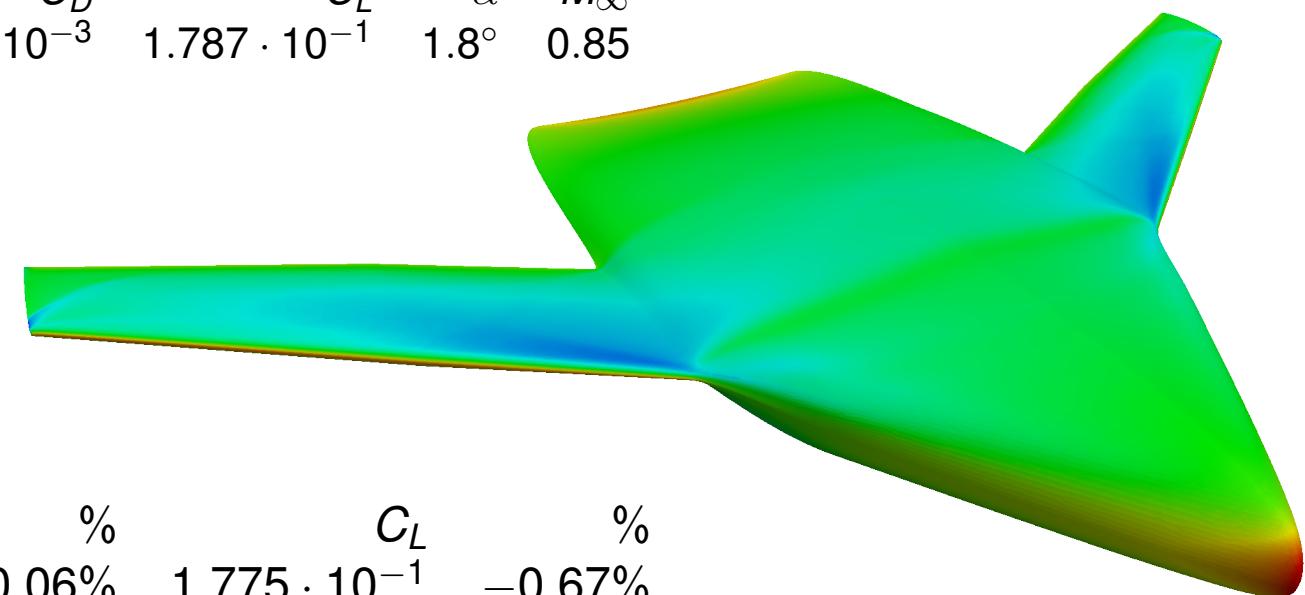
- 115,673 surface node positions to be optimised
- Planform constant

One-Shot Optimization of VELA (DLR)



[Schmidt, Schulz, Ilic, Gauger, 2011]

Shape	State	C_D	C_L	α	M_∞
115,673	29,297,175	$4.770 \cdot 10^{-3}$	$1.787 \cdot 10^{-1}$	1.8°	0.85



Shape	C_D	%	C_L	%
115,673	$3.342 \cdot 10^{-3}$	-30.06%	$1.775 \cdot 10^{-1}$	-0.67%

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- **Adjustments for Optimization with Unsteady PDEs**
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Problem Setup (Unsteady PDE)

Goal:

$$\min_{y,u} \frac{1}{T} \int_0^T f(y(t), u) dt \quad \text{subject to}$$

$$\frac{\partial y(t)}{\partial t} + c(y(t), u) = 0 \quad \forall t \in [0, T]$$

$$y(0) = y_*^0$$

- ▶ Use existing, well-established simulation tools.
- ▶ Implicit time marching scheme:

$$\frac{y(t_i) - y(t_{i-1})}{t_i - t_{i-1}} + c(y(t_i), u) = 0$$

for each discrete time step $0 = t_0 < \dots < t_N = T$.

Solving the Unsteady PDE

Given: Fixed point iterator G to solve the residuum equations at each time step:

for $t_1 < \dots < t_N$:

iterate $y_{k+1}(t_i) = G(y_k(t_i), y_*(t_{i-1}), u) \xrightarrow{k \rightarrow \infty} y_*(t_i)$

- ▶ Contractivity: $\left\| \frac{\partial G(y(t_i), y(t_{i-1}), u)}{\partial y(t_i)} \right\| \leq \rho < 1$

How to incorporate design updates for One-Shot?

Prepare for One-Shot

Modification of time marching scheme:

iterate $k = 0, 1, \dots :$

$$\text{for } t_1 < \dots < t_N : y_{k+1}(t_i) = G(y_k(t_i), y_{k+1}(t_{i-1}), u) \quad (*)$$

- ▶ Update a complete trajectory within one iteration.
- ▶ Consider $y = (y(t_1), \dots, y(t_N)) = (y^1, \dots, y^N) \in (\mathbb{R}^m)^N$ then

iterate $k = 0, 1, \dots :$

$$y_{k+1} = H(y_k, u)$$

where H performs $(*)$.

Contractivity of H

- ▶ The Jacobian $\frac{\partial H(y, u)}{\partial y}$ is block-triangular:

$$\frac{\partial H(y, u)}{\partial y} = \begin{pmatrix} \partial_{y^1} G(y^1, y^0, u) & 0 & 0 \\ * & \ddots & 0 \\ * & * & \partial_{y^N} G(y^N, y^{N-1}, u) \end{pmatrix}$$

- ▶ Its spectral radius is bounded:

$$\text{spr} \left(\frac{\partial H(y, u)}{\partial y} \right) = \max_{i \in \{1, \dots, N\}} \text{spr} \left(\partial_{y^i} G(y^i, y^{i-1}, u) \right) \leq \rho < 1$$

$\implies H$ is **contractive**.

[Günther, Gauger, 2013]

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Discrete Unsteady Optimization Problem

Goal:

$$\min_{y,u} \frac{1}{N} \sum_{i=1}^N f(y^i, u) \quad \text{s.t.} \quad y = H(y, u)$$

- ▶ $y \in (\mathbb{R}^m)^N$ state variable, $u \in \mathbb{R}^n$ design variable
- ▶ Fixed point iterator H to solve the unsteady PDE

$$y_{k+1} = H(y_k, u) \xrightarrow{k \rightarrow \infty} y_* = H(y_*, u)$$

- ▶ Contractivity: $\left\| \frac{\partial H}{\partial y} \right\| \leq \rho < 1$

⇒ Same structure as in steady case.

⇒ One-Shot method can be applied.

[Günther, Gauger, 2013]

Unsteady One-Shot Iterations

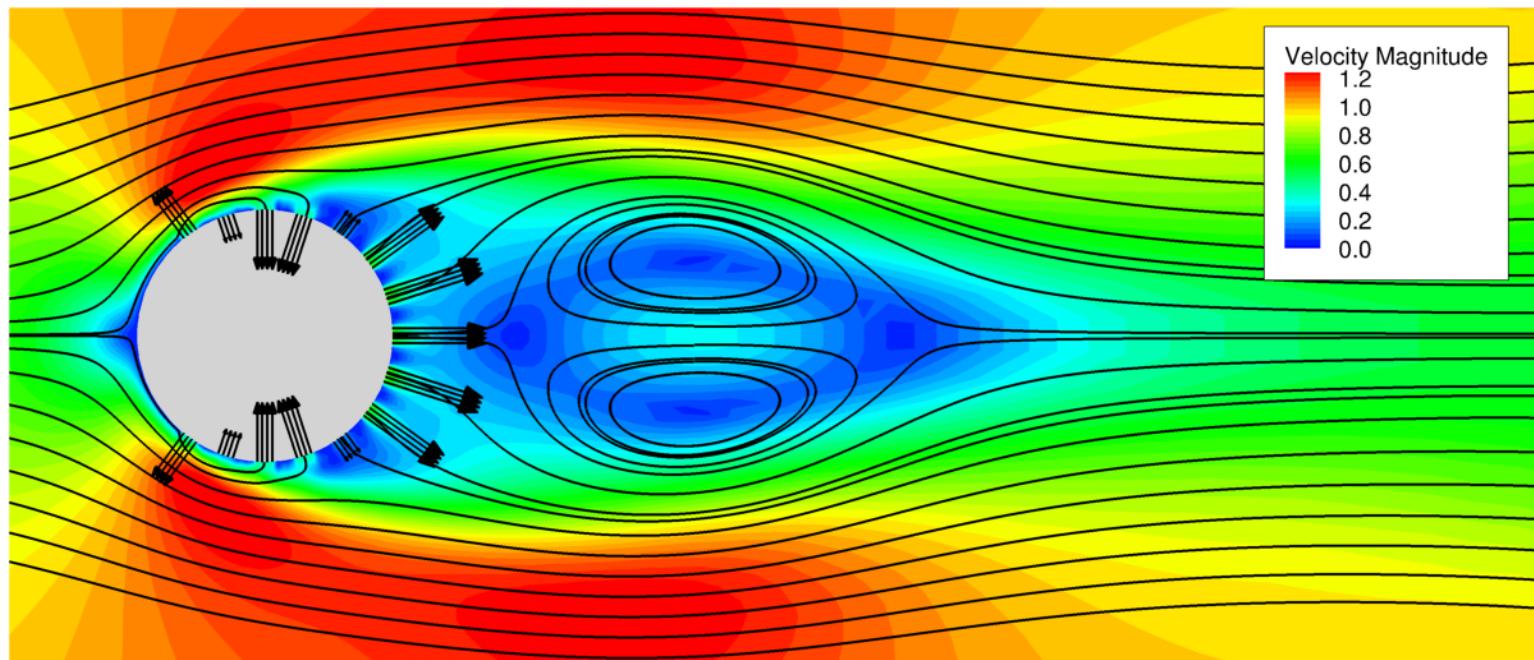
- ▶ Lagrangian function $L(y, \bar{y}, u) = J(y, u) + (H(y, u) - y)^T \bar{y}$
- ▶ Iterate simultaneously

$$\begin{bmatrix} y_{k+1} \\ \bar{y}_{k+1} \\ u_{k+1} \end{bmatrix} = \begin{bmatrix} H(y_k, u_k) \\ \nabla_y J(y_k, u_k) + H_y(y_k, u_k)^T \bar{y}_k \\ u_k - B_k^{-1} (\nabla_u J(y_k, u_k) + H_u(y_k, u_k)^T \bar{y}_k) \end{bmatrix}$$

- ▶ y_{k+1} contains loop over all time steps forward in time
- ▶ \bar{y}_{k+1} contains loop over all time steps backwards in time

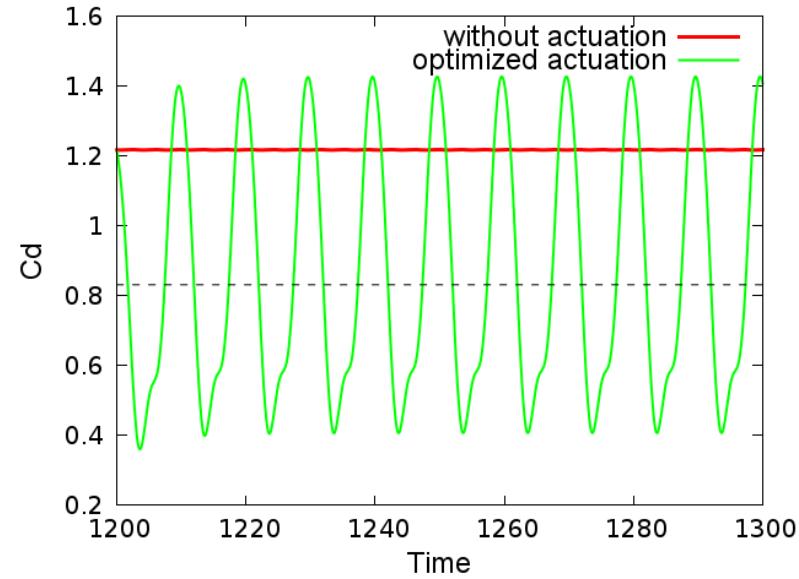
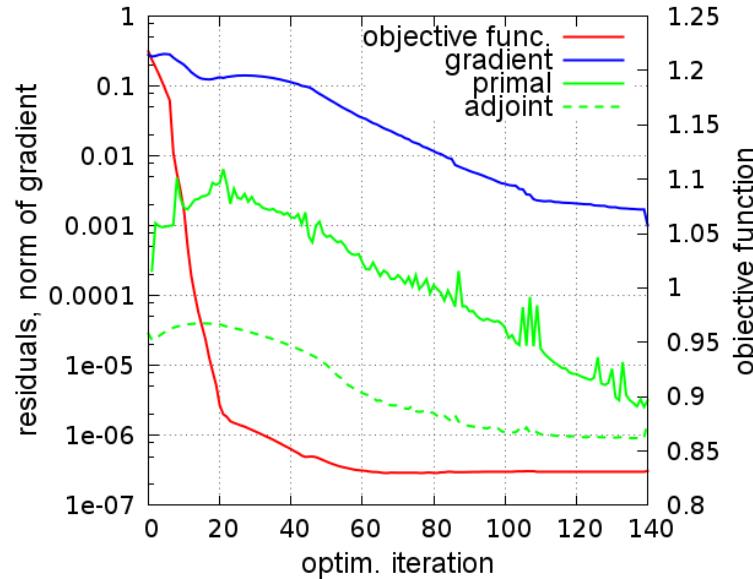
Optimal Active Flow Control

- ▶ Flow around cylinder at $Re=100$ governed by incompressible unsteady Reynolds-averaged Navier-Stokes equations (URANS)
- ▶ 15 actuation slots for pulsed blowing/suction
- ▶ Design parameters: Amplitude at each slot
- ▶ Objective function: Average drag coefficient



Unsteady One-Shot Optimization for Cylinder Flow

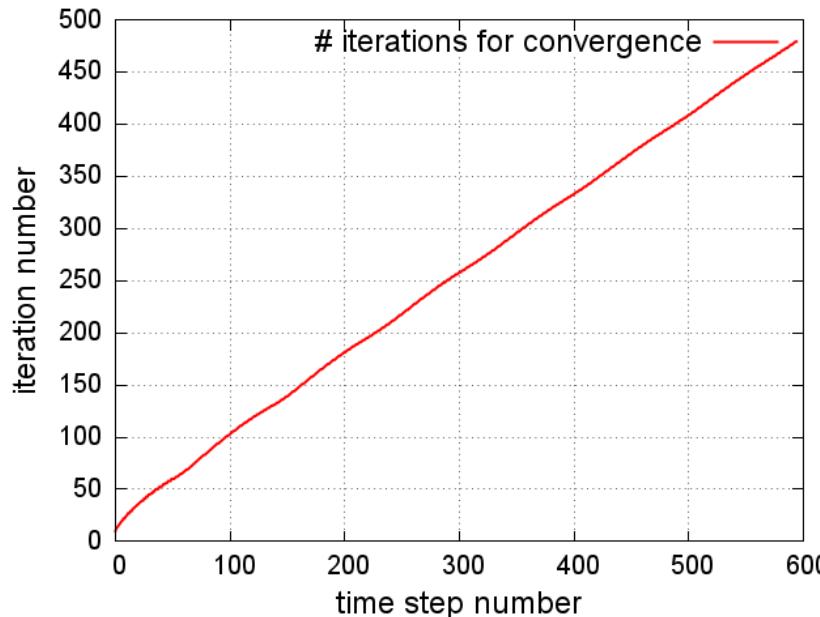
- ▶ Flow Solver ELAN (developed at ISTA, TU Berlin)
- ▶ Implicit 2nd order in space and time
- ▶ Pressure correction loops in each time step (SIMPLE algorithm)
- ▶ Modification for One-Shot framework
- ▶ Automatic Differentiation for generation of adjoint solver



[Günther, Gauger, Wang, 2015]

Efficiency of Unsteady One-Shot Approach?

- ▶ Bounded retardation for One-Shot applications
- ▶ Performance of modified time-marching scheme:



- ▶ Number of outer iteration cycles for primal convergence depends linearly on N .
- ▶ Each iteration cycle contains a loop over entire time domain.

Outline

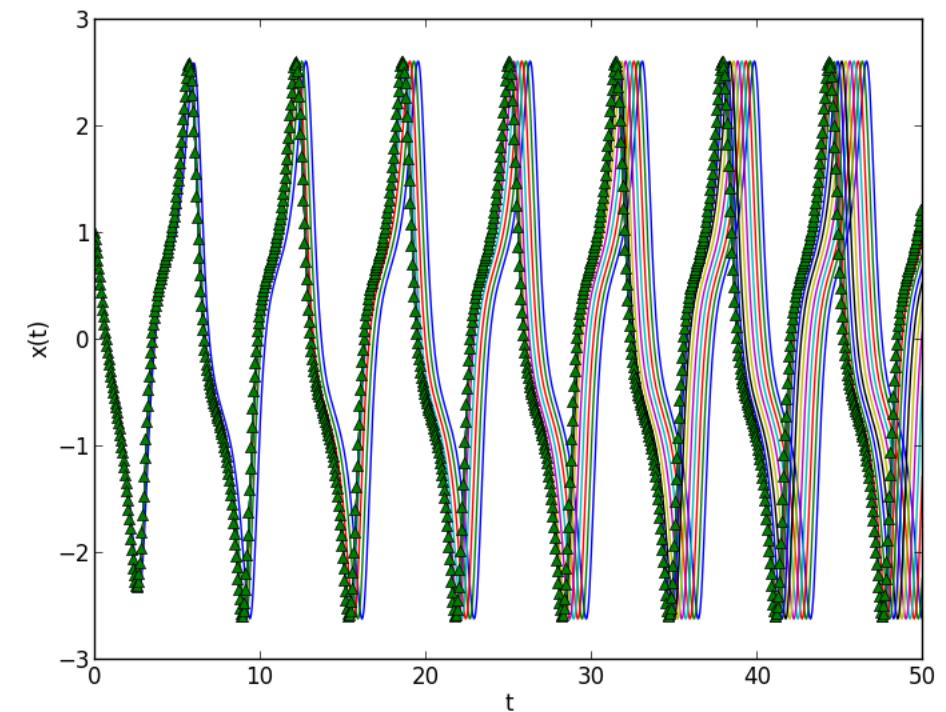
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Model Problem: Van der Pol Oscillator

$$\begin{pmatrix} \dot{x}(t) \\ \dot{v}(t) \end{pmatrix} = \begin{pmatrix} v(t) \\ -x(t) + u(1 - x(t)^2)v(t) \end{pmatrix} \quad \forall t \in [0, T]$$

$$\begin{pmatrix} x(0) \\ v(0) \end{pmatrix} = \begin{pmatrix} x_0 \\ v_0 \end{pmatrix}$$

- ▶ Autonomous ODE system
- ▶ Backward Euler discretization
- ▶ Quasi-Newton fixed point solver
- ▶ Modification for One-Shot framework
- ▶ **Numerical time dilation is the main error source.**



Adaptive Time Scaling

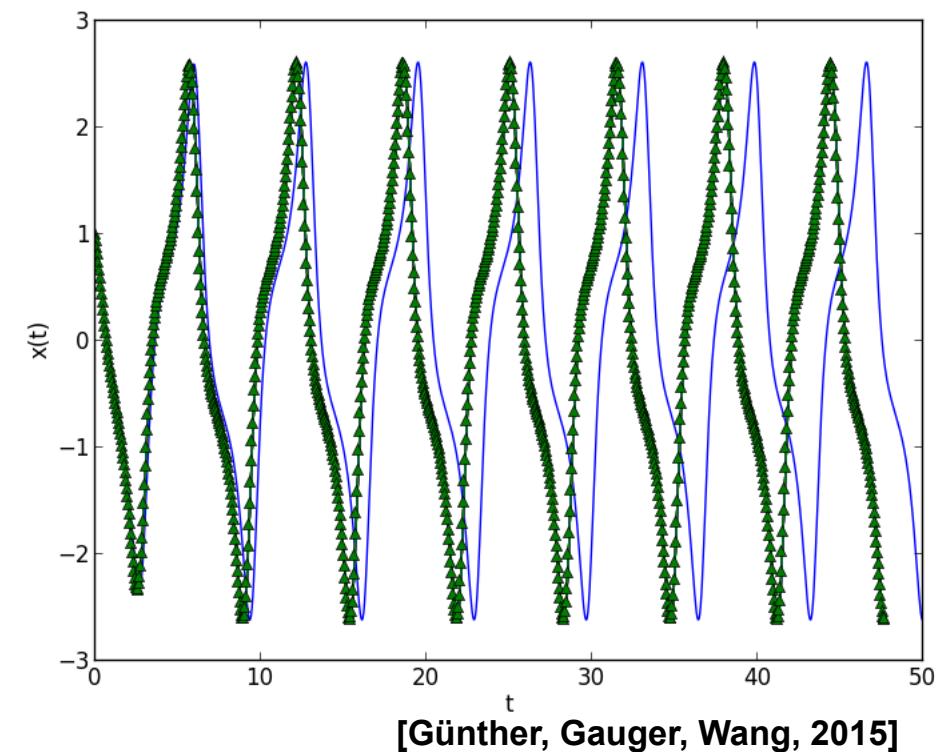
- ▶ Assign $\tilde{y}(t_i) := y(\tilde{t}_i)$ where \tilde{t}_i minimizes the residuum equation

$$\min_{\tilde{t}_i} \left\| \frac{y(t_i) - y(t_{i-1})}{\tilde{t}_i - t_{i-1}} + c(y(t_i), u) \right\|_2^2$$

- ▶ For autonomous ODEs:

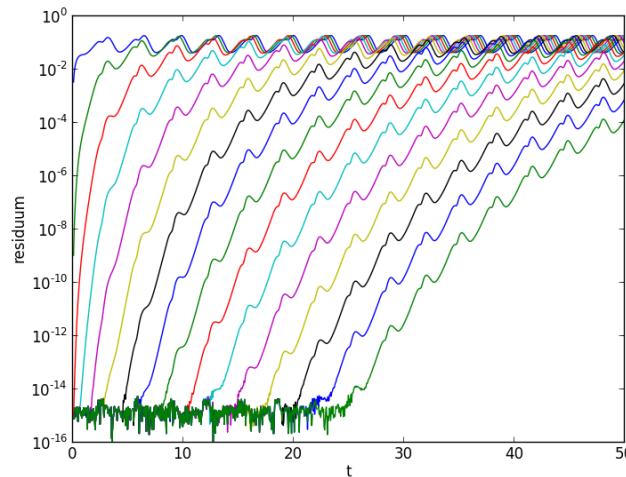
$$\tilde{t}_i = t_{i-1} - \frac{\langle y(t_i) - y(t_{i-1}), c(y(t_i), u) \rangle}{\|c(y(t_i), u)\|_2^2}$$

- ▶ **New trajectories are in phase with the unsteady solution.**

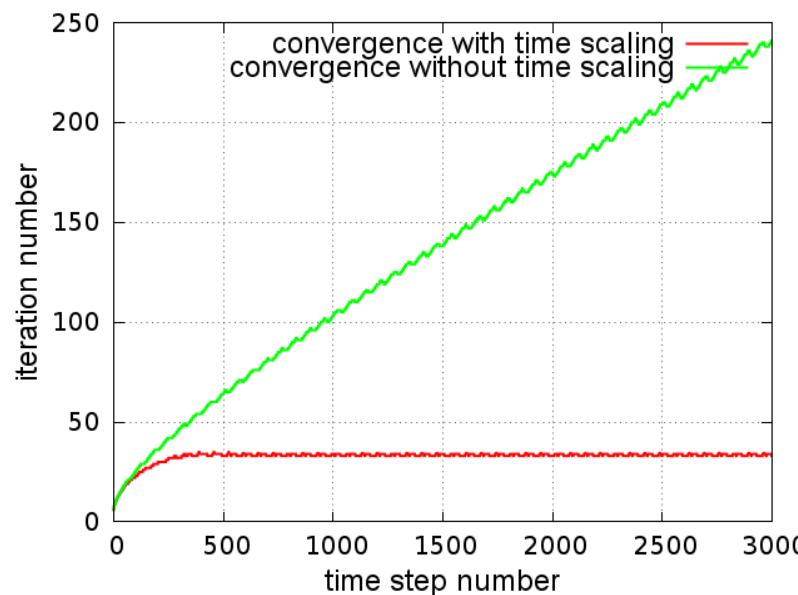
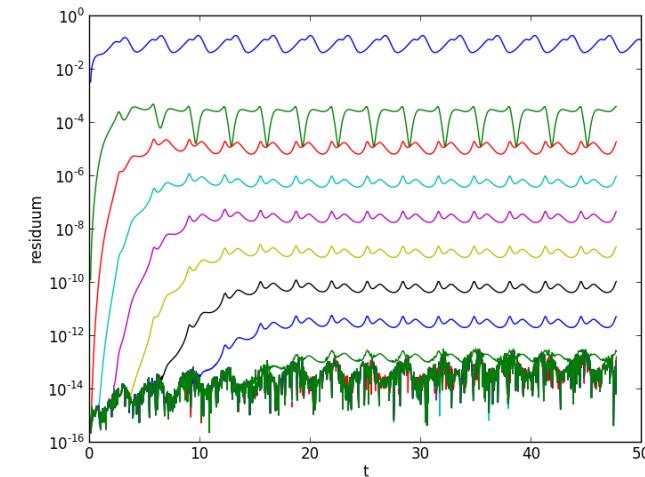


Adaptive Time Scaling

Residuals without time scaling



Residuals with time scaling



- ▶ Independence of number of time steps

[Günther, Gauger, Wang, 2015]

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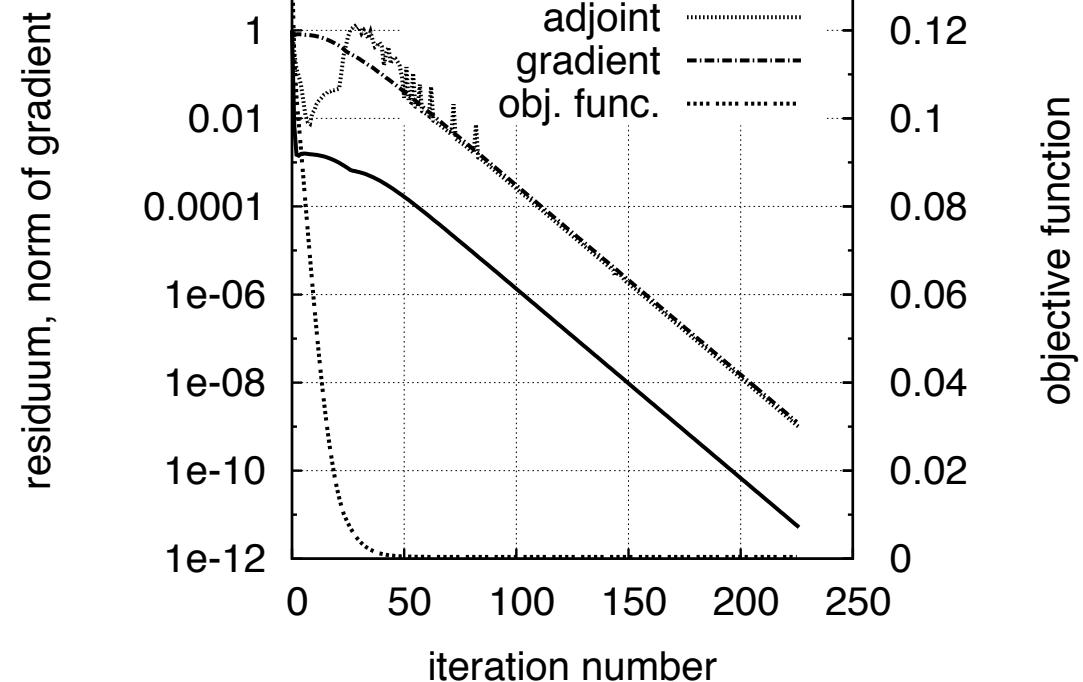
One-Shot Optimization

$$\min_{\mu, y} \int_0^T \|y - y_{ref}\|^2 + \gamma \|\mu\|^2 dt \quad \text{s.t.}$$

$$\begin{pmatrix} \dot{x}(t) \\ \dot{v}(t) \end{pmatrix} = \begin{pmatrix} v(t) \\ -x(t) + \mu (1 - x(t)^2) v(t) \end{pmatrix} \quad \forall t \in [0, T]$$

$$\begin{pmatrix} x(0) \\ v(0) \end{pmatrix} = \begin{pmatrix} x_0 \\ v_0 \end{pmatrix}$$

- ▶ BFGS-updates for the preconditioner
- ▶ Retardation factor = 7



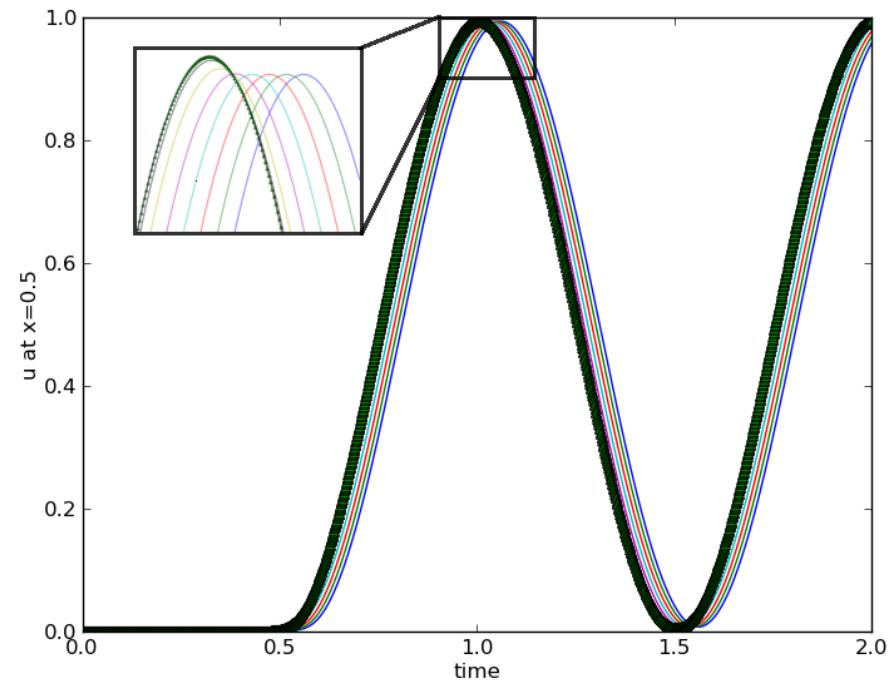
[Günther, Gauger, Wang, 2015]

Advection-Diffusion Equation

$$\begin{aligned}
 \dot{y}(t, x) + ay_x(t, x) - \mu y_{xx}(t, x) &= 0 & \forall x \in (0, 1), t > 0 \\
 y(t, 0) &= u \cdot (\sin(2\pi t) + 1) & \forall t > 0 \\
 y(0, x) &= 0 & \forall x \in [0, 1]
 \end{aligned}$$

with $a = 1.0$ and $\mu = 10^{-5}$.

- ▶ Non-autonomous ODE
- ▶ Backward Euler discretization
- ▶ Quasi-Newton fixed point solver
- ▶ Modification for One-Shot framework



- ▶ Numerical time dilation plus error in amplitude

Transformation into Autonomous System

- ▶ Transform non-autonomous PDE into a system of autonomous PDEs
- ▶ State $w(t) = (y(t), \mathbf{s}(t))$ satisfying

$$\begin{aligned}
 \dot{y}(t, x) + ay_x(t, x) - \mu y_{xx}(t, x) &= 0 & \forall x \in (0, 1), t > 0 \\
 y(t, 0) - u \cdot (\sin(2\pi \mathbf{s}(t)) + 1) &= 0 & \forall t > 0 \\
 y(0, x) &= 0 & \forall x \in [0, 1] \\
 \dot{\mathbf{s}}(t) &= 1 & \forall t > 0 \\
 s(0) &= 0
 \end{aligned}$$

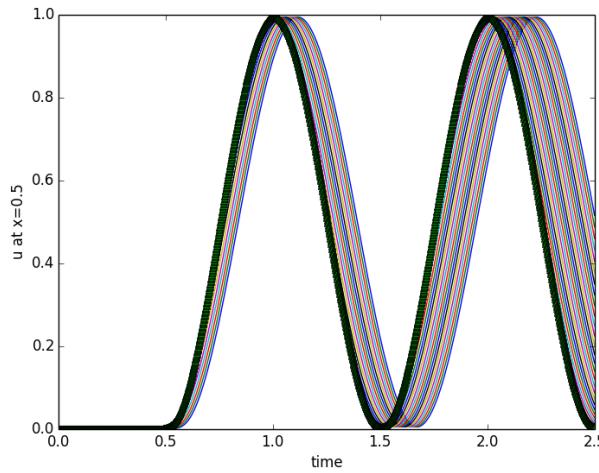
- ▶ Adaptive time scaling

$$\tilde{t}_i = t_{i-1} - \frac{\langle w(t_i) - w(t_{i-1}), c(w(t_i), u) \rangle}{\|c(w(t_i), u)\|_2^2}$$

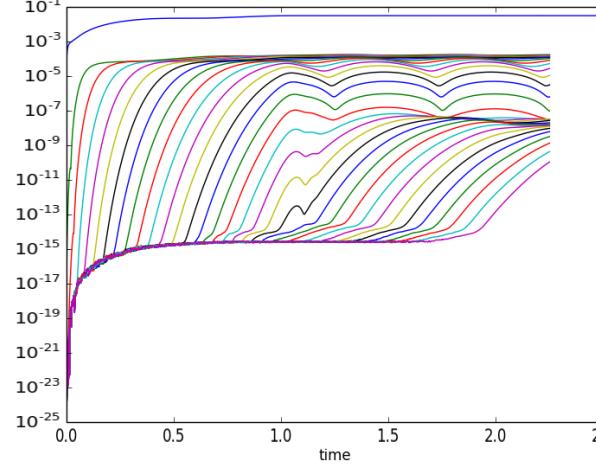
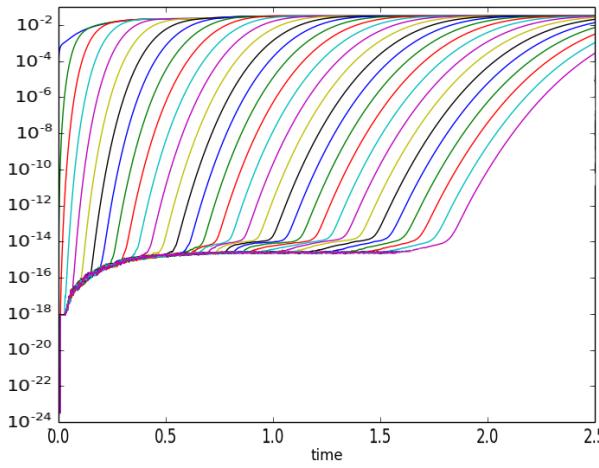
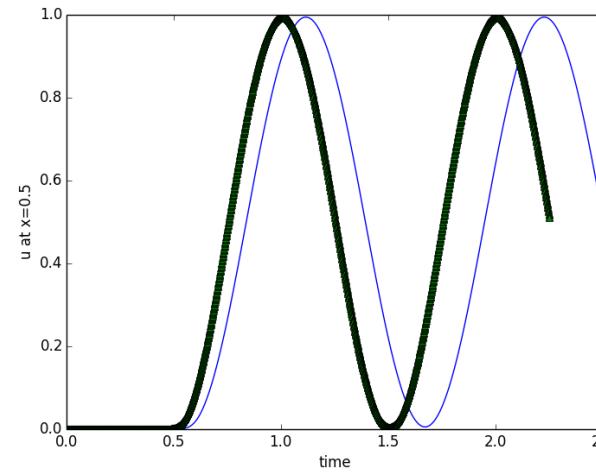
[Günther, Gauger, Wang, in prep.]

Adaptive Time Scaling

without time scaling



with time scaling



- ▶ Numerical time dilation eliminated

- ▶ Residual improvement by 5 orders of magnitude

[Günther, Gauger, Wang, in prep.]

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Thanks for your attention!