Scientific Computing

TECHNISCHE UNIVERSITÄT KAISERSLAUTERN

Semi-automatic transition from simulation to one-shot optimization with equality constraints

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September 15, 2016

AD 2016

Outline

Problem Definition

PDE-constrained optimization problem

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

$$\underset{\substack{\text{fixed point iteration} \\ ||G_y|| \leq \rho < 1}}{\longrightarrow}$$

$$\min_{u,y} \; f(y,u) \quad \text{s.t.} \; G(y,u) = y, \quad h(y,u) = 0$$

- objective function $f \in \mathbb{R}$, state $y \in Y \subset \mathbb{R}^n$, design $u \in U \subset \mathbb{R}^m$
- state equation $c : \; Y \times U \to Y$, constraints $h : Y \times U \to V \subset \mathbb{R}^p$ (notation: $\hat{G} = (G(y,u) - y, h(y,u))^T$)

$\Rightarrow$ one-shot approach using the AD-based discrete adjoint [Hamdi, Griewank(2010)],[Walther, Gauger, Kusch, Richert(2016)]

$$L(\bar{y}, y, u) = f(y,u) + (G(y,u) - y)^T \bar{y} + h^T \mu = N(y, \bar{y}, \mu, u) - y^T \bar{y}$$

The One-Shot Approach with Additional Constraints

KKT point (discrete)

$$
\begin{aligned}
y^* &= N_{\bar{y}}(y^*, \bar{y}^*, \mu, u^*)^T &&= G(y^*, u) \\
\bar{y}^* &= N_y(y^*, \bar{y}^*, \mu, u^*)^T &&= f_y(y^*, u^*)^T + G_y(y^*, u^*)^T \bar{y}^* \\
0 &= N_u(y^*, \bar{y}^*, \mu, u^*)^T &&= f_u(y^*, u^*)^T + G_u(y^*, u^*)^T \bar{y}^* \\
0 &= N_\mu(y^*, \bar{y}^*, \mu, u^*)^T &&= h(y^*, u^*)
\end{aligned}
$$

One-shot approach with equality constraints

for $k = 1, \ldots$

- $y_{k+1} = G(y_k, u_k)$
- $\bar{y}_{k+1} = N_y(y_k, \bar{y}_k, \mu_k, u_k)$
- $u_{k+1} = u_k - B_k^{-1} N_u(y_k, \bar{y}_k, \mu_k, u_k)$
- $\mu_{k+1} = \mu_k - \check{B}_k^{-1} h(y_k, u_k)$

Convergence Properties

doubly augmented Lagrangian

$$L^a(y, \bar{y}, \mu, u) = \frac{\alpha}{2}||\hat{G}(y, u)||^2 + \frac{\beta}{2}||N_y(y, \bar{y}, \mu, u)^T - \bar{y}||^2 + N - \bar{y}^T y$$

correspondence and descent condition

$$\sqrt{\alpha\beta}(1-\rho) > 1 + \frac{\beta}{2}||N_{yy}|| \quad (1)$$

and $\alpha \geq \|2(\hat{G}_u^\top)^{1\ldots p}(\hat{G}_y^\top)^+(N_{yu})_{1\ldots p} - (N_{uu})_{1\ldots p}^{1\ldots p}\|/\|(\hat{G}_u)_{1\ldots p}\|^2$

$\Rightarrow$ exact penalty function, descent for all large symmetric pos. def. B, $\check{B}$

choice of B

$B \approx \nabla^2_{uu} L^a(y, \bar{y}, u) \Rightarrow B = \alpha \hat{G}_u^T \hat{G}_u + \beta N_{yu}^T N_{yu} + N_{uu}$

Implementation Details

BFGS Update: $B\Delta u \approx \nabla_u L^a(y, \bar{y}, \mu, u + \Delta u) - \nabla_u L^a(y, \bar{y}, \mu, u) =: r$

calculate $\nabla_u L^a = \alpha \Delta y_k^T G_u + \alpha h_u^T h + \beta \Delta \bar{y}_k^T N_{yu} + N_u$

- N_u and $\Delta y_k^T G_u + h_u^T h$ can be obtained with reverse mode of AD from $\bar{u}$

$$\begin{aligned} y &= G(y, u) \\ v &= f(y, u) \\ w &= h(y, u) \end{aligned} \qquad \bar{u} = f_u(y, u)^T \bar{v} + G_u(y, u)^T \bar{y} + h_u(y, u)^T \bar{w}$$

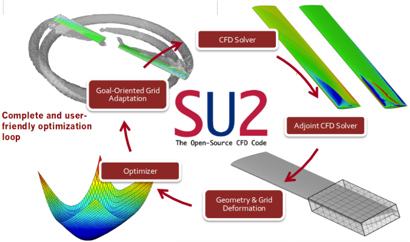
- finite difference over reverse / tangent over reverse

$$\Delta \bar{y}_k^T N_{yu} \approx \frac{1}{h} \left(N_u(y_k + h\Delta \bar{y}_k, \bar{y}_k, \mu_k, u_k) - N_u(y_k, \bar{y}_k, \mu_k, u_k) \right) \qquad (2)$$

- curvature condition: set $B_k = I$ if $r_k^T \Delta u_k \leq 0$

Open-source multiphysics suite SU2

- Under active development (Stanford University, TU Kaiserslautern, TU Delft,...)
- FV discretization of (U)RANS equations and turbulence models using highly modular C++ code-structure, additional PDE solvers
- Multi-grid and local time-stepping methods
- Several space and time discretizations, MPI, python scripts
- optimization environment based on continuous or discrete adjoint, integrated AD support [Albring, Sagebaum, Gauger(2015)]



Discrete-Adjoint Solver in SU2

- operator overloading (frequent extensions/improvements)
- shape optimization → mesh deformation as additional constraint in the optimization problem $M(u) = x$
- fixed-point form $\bar{y}_{k+1} = N_y(y_k, \bar{y}_k, \mu_k, u_k)^T$

CoDiPack

- open-source (https://github.com/SciCompKL/CoDiPack)
- use of expression templates
- different tape implementations

Performance SU2 (NASA Common Research Model)

- Runtime Factor: 1.2
- Memory Factor: 7.2

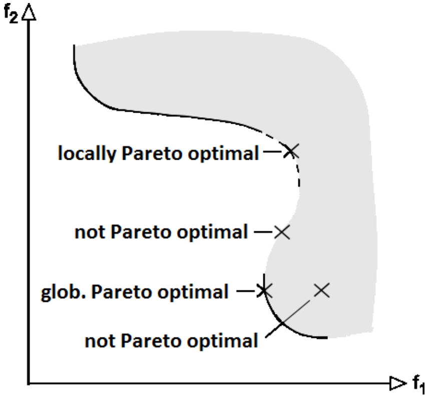
Multi-Objective Optimization Problem

$$\min_{y,u} \quad \mathbf{F}(y,u)$$
$$\text{s.t.} \quad c(y,u) = 0, \tag{3}$$
$$h(y,u) \geq 0 \tag{4}$$

Pareto dominance:

$\overline{x}$ dominates x if

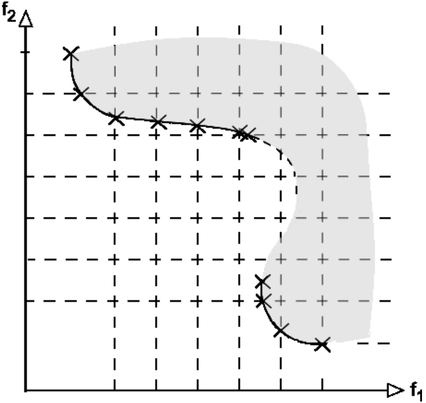
$$\forall i \in \{1,...,k\} : \quad f_i(\overline{x}) \leq f_i(x)$$
$$\exists j \in \{1,...,k\} : \quad f_j(\overline{x}) < f_j(x)$$



Methods for Multi-Objective Optimization

- common: weighted sum, evolutionary algorithms
- ε-constraint method [Marglin(1967)]

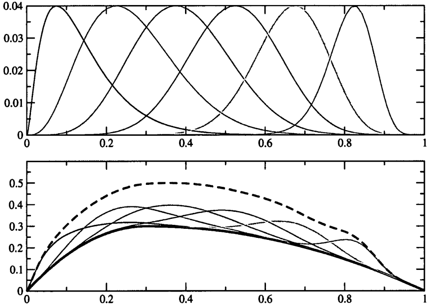
$$\begin{aligned} \min_{y,u} \quad & f_{s_j}(y,u) \\ \text{s.t.} \quad & c(y,u) = 0, \\ & h(y,u) = 0, \\ & f_i(x) \leq f_i^{(j)} \\ & \forall\ i \in \{1, ..., k\} \quad i \neq s_j \end{aligned} \tag{5}$$



- connected: equality constraints

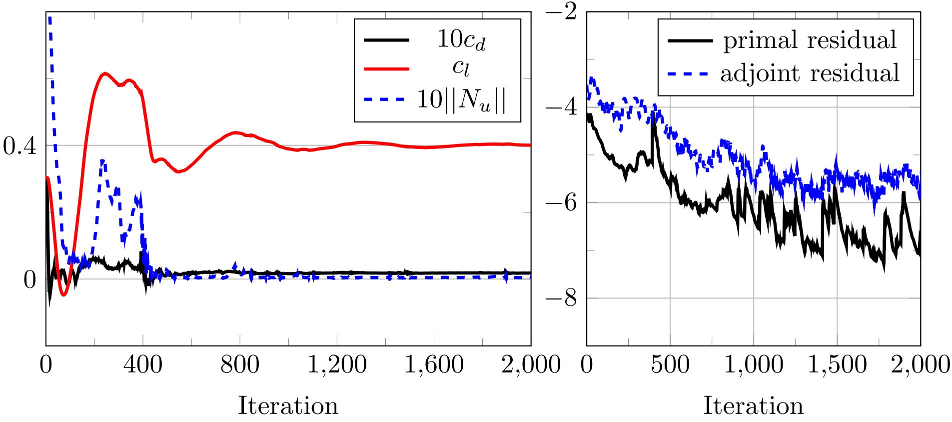
Application (Airfoil Design)

- aerodynamic shape optimization of NACA 0012 airfoil
- objectives: drag coefficient c_d, lift coefficient c_l
- bounded design variables: 38 Hicks-Henne bump functions (bounds: [-0.005,0.005])
- constraints: moment, thickness
- steady Euler equations, transonic flow (Mach 0.8 and AOA 1.25)

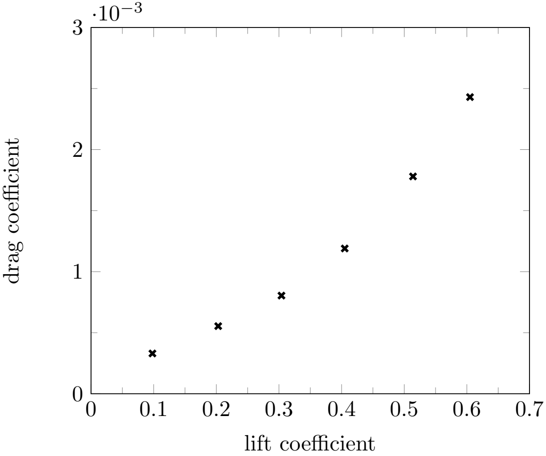


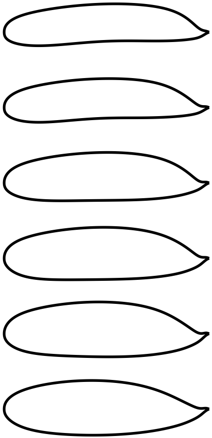
Result: Lift Constraint

preconditioner $\check{B} = 20$, $\mu_0 = 0$, target lift: 0.4
backtracking line search, trial step size: 1, $\alpha = 20$, $\beta = 2$



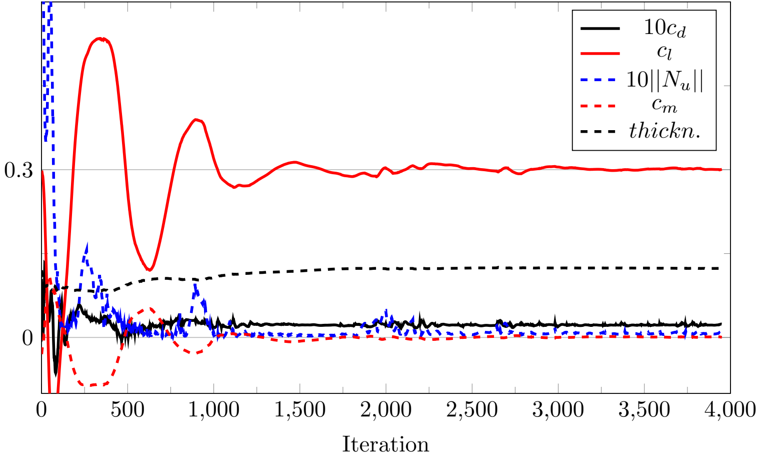
Resulting Pareto-optimal Front



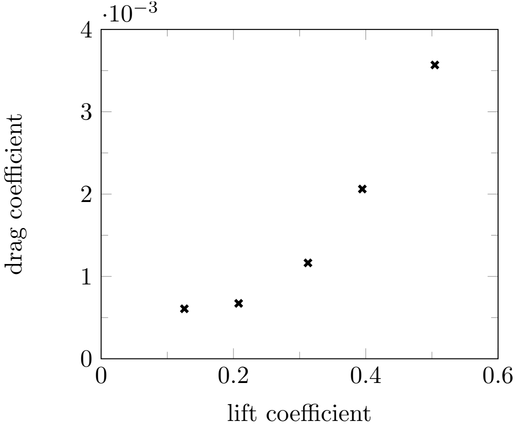


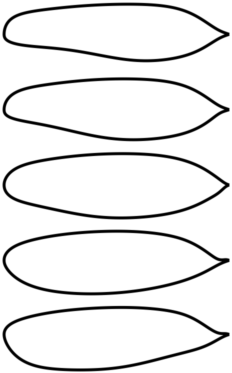
Result: Lift, Moment, Thickness Constraint

target lift: 0.3, moment: 0.0, thickness: 0.12
preconditioner diag(20, 20, 100), $\mu_{i,0} = 0$



Resulting Pareto-optimal Front





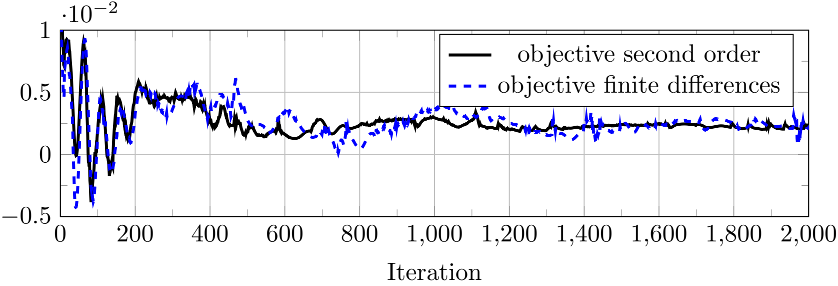
Using Second-Order Adjoints

Tangent over Reverse: $\Delta \bar{y}_k^T N_{yu}$

$$\dot{\bar{u}}^T = (\bar{y}^T G_{uy} + \bar{v}^T f_{yu} + \bar{w}^T h_{yu})\dot{y} + \text{other terms} \tag{6}$$

$\Rightarrow$ Set $\bar{v} = 1$, $\bar{w} = \mu$, $\bar{y} = \bar{y}$, $\dot{y} = \Delta\bar{y}$, Read from $\dot{\bar{u}}$ (Runtime Factor: 1.6)

DataType: `ActiveReal<RealForward, ChunkTape<RealForward, int>>`
GetMixedDerivative: `tape.getGradient(x[adjPos++]).getGradient()`



Summary and Outlook

Summary

Semi-automatic transition from simulation to optimization involving

- AD-based discrete adjoint in SU2
- constrained one-shot method and
- deterministic multi-objective optimization

Outlook

- different application in SU2 (multi-disciplinary)
- investigations on preconditioner for constraints

Thank you for your attention!

References

Hamdi, A. and Griewank, A.
Properties of an augmented lagrangian for design optimization.
Optimization Methods and Software **25**(4), 645–664 (2010).

Walther, A., Gauger, N., Kusch, L., and Richert, N.
On an extension of one-shot methods to incorporate additional constraints.
Optimization Methods and Software (2016).

Albring, T., Sagebaum, M., and Gauger, N.
Development of a consistent discrete adjoint solver in an evolving aerodynamic design framework.
AIAA 2015-3240 (2015).

Marglin, S. A.
Public investment criteria.
Allen & Unwin London, (1967).