Large Scale Shape Optimization in CFD

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Outline

Optimization Algorithm

One-Shot: Approximative reduced SQP method with inexact gradients:

1. Perform n_u flow solver steps for state u
2. Perform n_{λ_d} steps of the adjoint flow solver w.r.t. drag
3. Perform n_{λ_ℓ} steps of the adjoint flow solver w.r.t. lift
4. Compute approximation B of the reduced Hessian
5. Solve

$$\begin{bmatrix} B & \tilde{D}_\ell \\ \tilde{D}_\ell^T & 0 \end{bmatrix} \begin{pmatrix} \Delta q \\ \nu_{k+1} \end{pmatrix} = \begin{pmatrix} -\tilde{D}_f \\ \lambda_\ell c - \ell \end{pmatrix}$$

   with $\tilde{D}_f = \nabla_q f - (D_q c)^T (D_u c)^{-T} \nabla_u f$

6. Set $q_{k+1} = q_k + \tau \Delta q$
7. Adapt CFD mesh and goto 1.

Crucial: Fast gradient evaluation, good Hessian approximation

Standard Parametric Paradigm

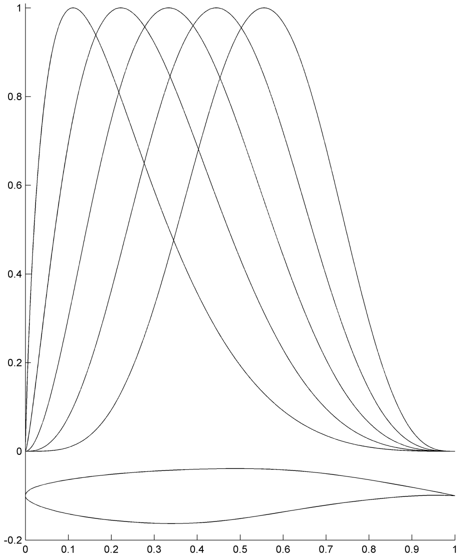
- Choose fixed geometry parametrization $q \in \mathbb{R}^{n_q}$
- Results in finite dimensional NLP:

$$\min_q F(u(q), q)$$

- Gradient given by formal Lagrangian for finite dimensional problem:

$$\frac{dF}{dq}(u(q), q) = \frac{\partial F}{\partial q} - \lambda^T \frac{\partial c}{\partial q}$$

$$\left[\frac{\partial c}{\partial u}\right]^T \lambda = \frac{\partial F}{\partial u}$$



Shape Optimization Paradigm

- One parametric family of bijective mappings:

$$T_t : \mathbb{R}^n \to \mathbb{R}^n \; \forall t \in [0, \tau], \quad (t, x) \mapsto T_t(x)$$
$$\Omega_t := T_t(\Omega) = \{T_t(x_0) \mid x_0 \in \Omega\}$$

- Speed Method: T_t defined via "flow equation":

$$\frac{dx}{dt} = V(t, x), \; x(0) = x_0$$

- Perturbation of identity:

$$T_t(x_0) = x_0 + tV(x_0)$$

Shape Derivative

$$dJ[V] := \lim_{t \to 0^+} \frac{J(\Omega_t) - J(\Omega)}{t}$$

Shape Derivative

Objective Function

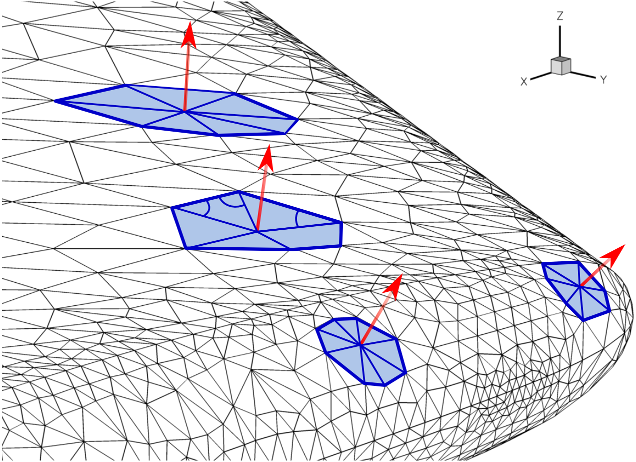
$$J(\Omega_t) := \int_{\Gamma_t} h(x)\, d\lambda_t^{n-1}(x) = \int_{\Gamma} h(T_t(x))\, d\lambda_t^{n-1}(x)$$

$$= \int_{\Gamma} h(T_t(x)) \det(DT_t(x)) \| DT_t^{-*}(x) n(x) \|\, d\lambda^{n-1}(x)$$

Shape Derivative

$$dJ(\Omega)[V] = \int_{\Gamma} \langle \nabla_x h, V \rangle + h[\operatorname{div} V - \langle DVn, n \rangle]\, d\lambda^{n-1}$$

Shape Optimization Paradigm



- Choose V_i as hat-function over surface node p_i
- Each node of the wing is design parameter
- Must be computable in one sweep

The Hadamard Theorem (cf. Sokolowski, Zolésio, 1992)

Under some regularity assumptions, there exists a scalar distribution $G(\Gamma)$ with support on Γ such that

$$dJ(\Omega)[V] = \langle G(\Gamma), \langle V, n \rangle \rangle = \int_\Gamma \langle V, n \rangle \, g \, dS$$

Shape Derivative is a scalar product with direction $\langle V, n \rangle$

Shape Derivative with Hadamard Theorem

$$J(\Omega) = \int_\Gamma h \, d\lambda^{n-1}$$

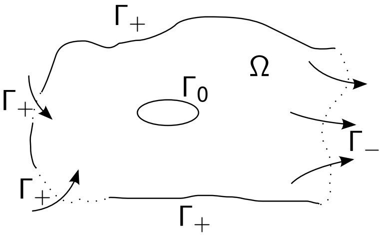
$$dJ(\Omega)[V] = \int_\Gamma \langle V, n \rangle \, \left[\frac{\partial h}{\partial n} + \kappa \, h \right] \, d\lambda^{n-1}$$

Model Problem: Incompressible Navier–Stokes

$$\min_{(u,p,\Omega)} J(u,p,\Omega) := \int_\Omega f(u, Du, p)\, dA + \int_{\Gamma_0} g(u, D_n u, p, n)\, dS$$

subject to

$$
\begin{aligned}
-\mu\Delta u + \rho u \nabla u + \nabla p &= \rho G \quad \text{in} \quad \Omega \\
\operatorname{div} u &= 0 \\
u &= u_+ \quad \text{on} \quad \Gamma_+ \\
u &= 0 \quad \text{on} \quad \Gamma_0 \\
pn - \mu \frac{\partial u}{\partial n} &= 0 \quad \text{on} \quad \Gamma_-
\end{aligned}
$$



- $f : \mathbb{R}^d \times \mathbb{R}^{d\times d} \times \mathbb{R} \to \mathbb{R}$, $(u, C, p) \mapsto f(u, C, p)$
- $g : \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}$, $(u, b, p, n) \mapsto g(u, b, p, n)$

Shape Derivative

$$
\begin{aligned}
&dJ(u,p,\Omega)[V] = \\
&\int_{\Gamma_0} \langle V,n\rangle f(u,Du,p)\; dS \\
&+ \int_{\Gamma_0} \langle V,n\rangle \left[D_{(u,b,p)} g(u,D_n u,p,n)\cdot n + \kappa g(u,D_n u,p,n)\right]\; dS \\
&+ \int_{\Gamma_0} \langle V,n\rangle \left[-\sum_{i=1}^{d}\left(\frac{\partial g}{\partial u_i} + \mu\frac{\partial \lambda_i}{\partial n} + \sum_{j=1}^{d}\frac{\partial f}{\partial c_{ij}} n_j\right)\frac{\partial u_i}{\partial n}\right]\; dS \\
&+ \int_{\Gamma_0} \langle V,n\rangle \left[(\operatorname{div}_\Gamma \nabla_n g) - \kappa\langle \nabla_n g, n\rangle\right]\; dS
\end{aligned}
$$

Possible Objective Functions

Fluid Energy Dissipation into Heat

$$\min_{(u,p,\Omega)} \dot{E}(u,\Omega) := \frac{1}{2}\int_{\Omega} \mu \sum_{j,k=1}^{3} \left(\frac{\partial u_k}{\partial x_j}\right)^2 dA$$

Aerodynamic Drag

$$\min_{(u,p,\Omega)} F_D := \int_{\Gamma_0} -\mu \left\langle D_n u, a \right\rangle + p\langle n, a\rangle \; dS$$

Fluid Energy Dissipation: First Order Shape Calculus

a) Stokes

$$d\dot{E}_S(u,\Omega)[V] = \int_\Gamma \langle V, n\rangle \left[-\mu \sum_{k=1}^{3} \left(\frac{\partial u_k}{\partial n}\right)^2\right] dS$$

b) Navier–Stokes

$$d\dot{E}_{NS}(u,\Omega)[V] = \int_\Gamma \langle V, n\rangle \left[-\mu \sum_{k=1}^{3} \left(\frac{\partial u_k}{\partial n}\right)^2 - \frac{\partial u_k}{\partial n}\frac{\partial \lambda_k}{\partial n}\right] dS$$

$$\begin{aligned} -\mu\Delta\lambda - \rho\lambda\nabla u - \rho\,(\nabla\lambda)^T u + \nabla\lambda_p &= -2\Delta u \quad \text{in } \Omega \\ \text{div } \lambda_p &= 0 \quad \text{in } \Omega \end{aligned}$$

Second Order Shape Calculus

$$d^2 \dot{E}_S(u, \Omega)[V, W] = I_1 + I_2$$

where

$$I_1 = \int_\Gamma \langle W, n \rangle \left[\text{div } V \left(-\mu \sum_{i,j=1}^{3} \left(\frac{\partial u_i}{\partial x_j} \right)^2 \right) + V_\Gamma \nabla \left(-\mu \sum_{i,j=1}^{3} \left(\frac{\partial u_i}{\partial x_j} \right)^2 \right) \right]$$

$$I_2 = \int_\Gamma \langle V, n \rangle \left[2\mu \sum_{i=1}^{3} \frac{\partial u_i}{\partial n} S \left(\frac{\partial u_i}{\partial n} \langle W, n \rangle \right) \right]$$

$$+ \langle W, n \rangle \langle V, n \rangle \frac{\partial}{\partial n} \left(-\mu \sum_{i,j=1}^{3} \left(\frac{\partial u_i}{\partial x_j} \right)^2 \right)$$

- Divergence-free Poincaré-Steklov operator S
- Not computable in one sweep

Symbol of an Operator

Suppose Fourier disturbance (oscillation) of design: $\tilde{q}(x) = e^{i\omega x}$

- First order differential operator: $H\tilde{q} = i\omega\tilde{q}$
- Second order differential operator: $H\tilde{q} = -\omega^2\tilde{q}$
- Dirichlet to Neumann Map / Poincaré-Steklov: $H\tilde{q} = |\omega|\tilde{q}$

Stokes (analytic) / Navier–Stokes (frequency analysis):

$$H\tilde{q} = (\beta \cdot |\omega| + \gamma)\tilde{q}$$

Approximation:

$$\tilde{H} = -\alpha\Delta_\Gamma + id$$

Symbol: $1 + \alpha\omega^2$

α chosen to match boundary discretization

Symbol of the Stokes Hessian

Variation in gradient and state given by

$$\delta G\tilde{q} = -2\mu \sum_{k=1}^{2} \frac{\partial u_k}{\partial x_2} \frac{\partial u_k'[\tilde{q}]}{\partial x_2}, \quad u_k'[\tilde{q}] = \hat{u}_k e^{i\omega_1 x_1} e^{\omega_2 x_2}$$

Boundary condition gives

$$\hat{u}_k = \frac{\partial u_i}{\partial x_2}$$

Divergence-Free Poincaré-Steklov in Fourier Space gives

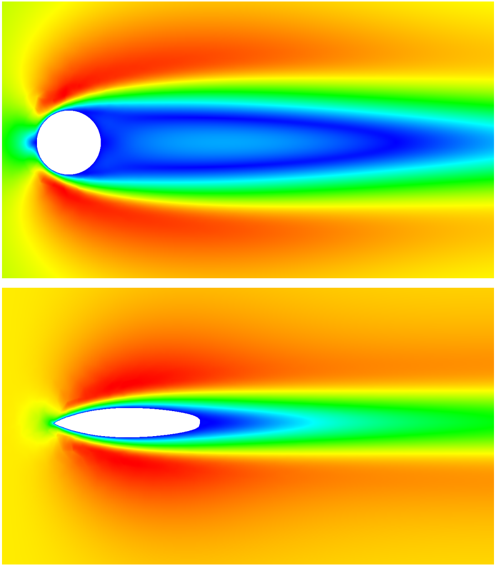
$$\begin{bmatrix} -\mu(-\omega_1^2 + \omega_2^2) & 0 & i\omega_1 \\ 0 & -\mu(-\omega_1^2 + \omega_2^2) & \omega_2 \\ i\omega_1 & \omega_2 & 0 \end{bmatrix} \begin{pmatrix} \hat{u}_1 \\ \hat{u}_2 \\ \hat{p} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Non-Contradiction

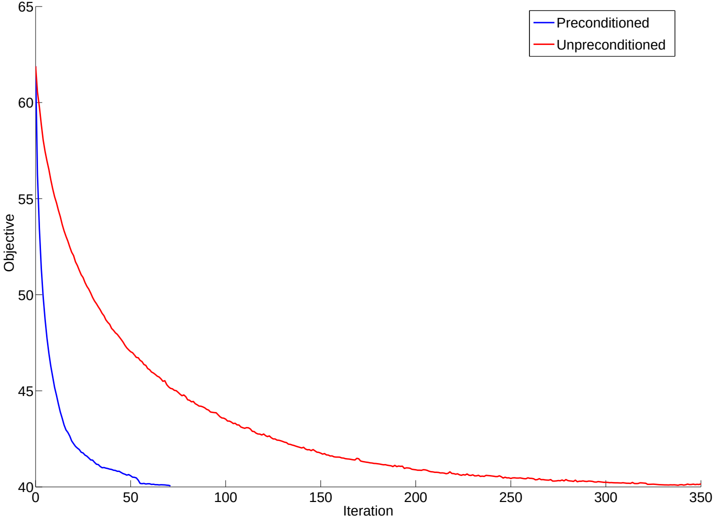
Only frequencies non-contradicting the above:

$$\omega_1 = |\omega_2|$$

Navier–Stokes: Initial and Optimal Domain



Performance: Navier–Stokes



- Optimum in iteration 71 vs 350: 80% less iterations

Euler Drag Reduction

Minimize Wave Drag

$$\min_{(u,\Omega)} J(u,\Omega) := \int_\Gamma \langle p_\ell, n\rangle \, dS = \int_\Gamma p \cdot n_\ell \, dS$$

subject to

$$0 = A_1(V)\frac{\partial U}{\partial x_1} + A_2(V)\frac{\partial U}{\partial x_2} + A_3(V)\frac{\partial U}{\partial x_3} \quad \text{in } \Omega$$

$$0 = \langle u, n\rangle \quad \text{on } \Gamma$$

$$u_\infty = u \quad \text{on } \Gamma_{\text{inflow}}$$

- Euler Flux Jacobian: $A_i(V)$
- Conserved variables: $U = (\rho, \rho u_1, \rho u_2, \rho u_3, \rho E)^T$
- Primitive variables: $V = (\rho, u_1, u_2, u_3, p)^T$
- Perfect gas: $p = (\gamma - 1)\rho(E - \frac{1}{2}(u_1^2 + u_2^2 + u_3^2))$

Euler Gradient

Shape Derivative for Euler Drag Reduction

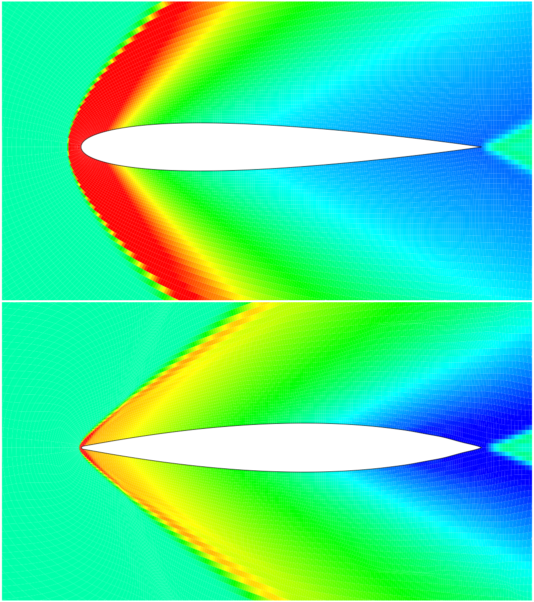
$$dF_\ell(\Omega)[V] = \int_\Gamma \langle V, n\rangle \left[\langle \nabla p_\ell \; n, n\rangle + \kappa \langle p_\ell, n\rangle - \lambda U_H \langle Du \cdot n, n\rangle\right] + (p_\ell - \lambda U_H u) dn[V] \; dS$$

$$= \int_\Gamma \langle V, n\rangle \left[\langle \nabla p_\ell \; n, n\rangle - \lambda U_H \langle Du \cdot n, n\rangle + \mathrm{div}_\Gamma \, (p_\ell - \lambda U_H u)\right]$$

- Hessian Symbol: 2D: $H\tilde{q} = -\omega^2 \tilde{q}$
  3D: $H\tilde{q} = -\frac{\omega_1^2}{\omega_2}\tilde{q}$ (cf. Arian, Ta'asan 1996), $H\tilde{q} = -(\omega_1^2 + \omega_2^2)\tilde{q}$ (here)
- MDO: Constraint on contour length and bending stiffness

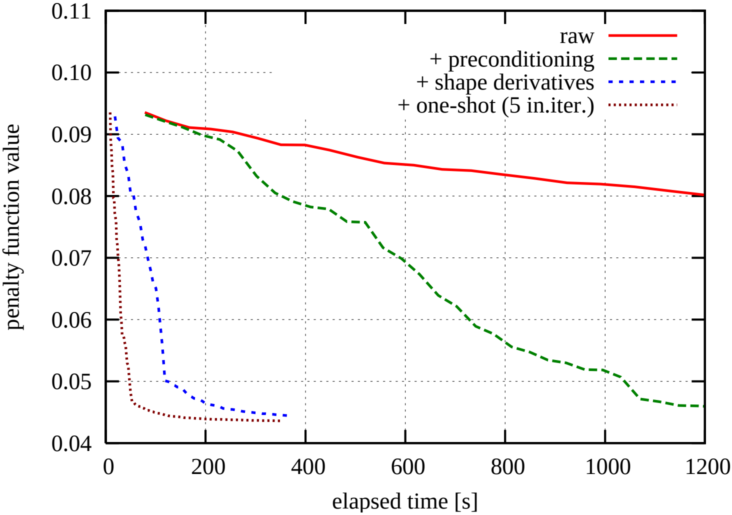
$$\int_\Gamma dS \leq L_0, \quad \int_\Gamma (y - y_c)^2 \; dS \geq I_{x_0}$$

Optimized Shape: Supersonic



- DLR Flow Solver TAU
- Unstructured Finite Volume
- Mach 2.00
- Initial NACA0012: $C_D = 9.430 \cdot 10^{-2}$
- Optimal Haack Ogive: $C_D = 4.721 \cdot 10^{-2}$
- Reduction by 49.9%
- 400 design parameters

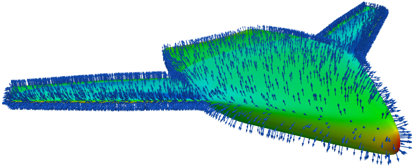
Optimization History: Wall-Clock-Time



Wall-clock time reduced by 99% (2.77h vs. 100s)

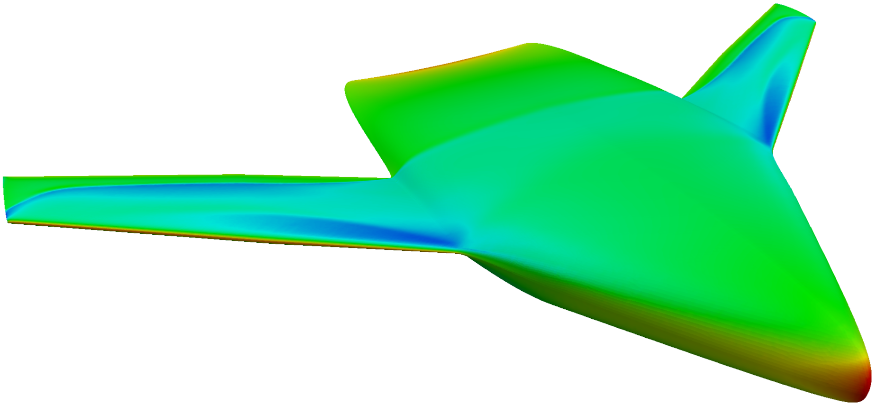
VELA Aircraft

VELA: Very Efficient Large Aircraft
Design study for blended wing-body configurations



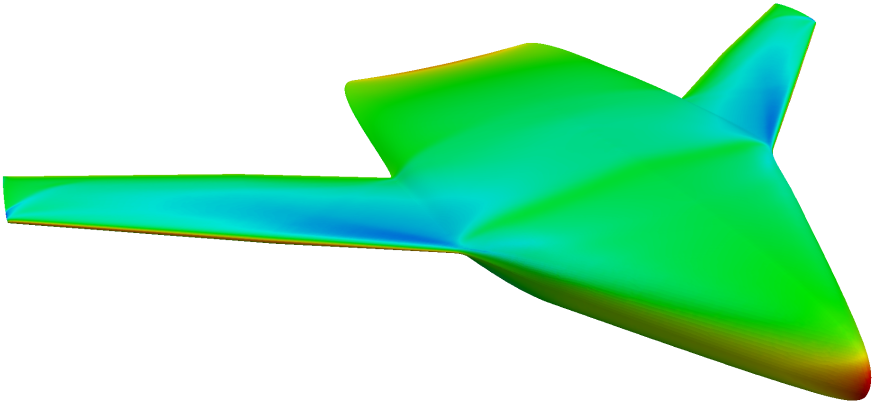
- $115,673$ surface node positions to be optimized
- Perturbation in initial normal direction: $V = n$
- Planform constant

3D Aircraft Optimization: VELA



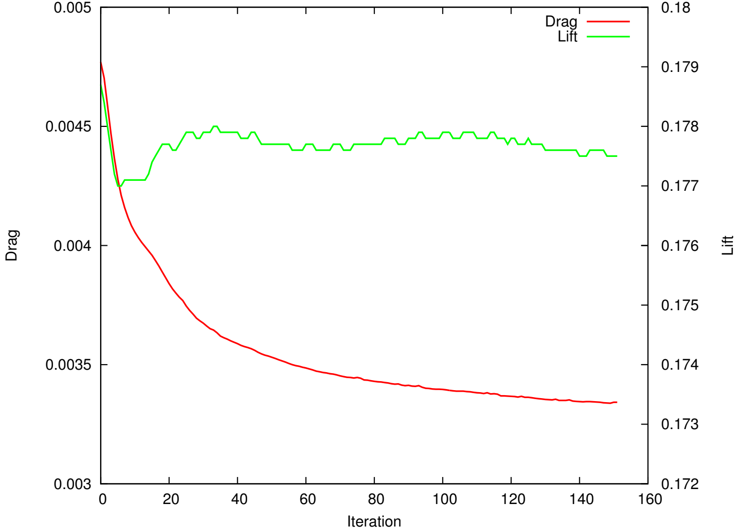
Shape	State	C_D	C_L	α	M_∞
115,673	29,297,175	$4.770 \cdot 10^{-3}$	$1.787 \cdot 10^{-1}$	1.8°	0.85

3D Aircraft Optimization: VELA



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

Convergence History



Conclusions

Summary:

- Derivation of shape gradients and Hessians
- Hessian operator symbol approximations
- Good Hessian approximation results in equation $\frac{\text{optimization}}{\text{simulation}} \approx 2.5$
- Structure exploitation CPU wall-clock time improvements:
  - Shape Hessian: 88%
  - Shape derivative: 75%

Conclusions:

- Structure exploitation of shape optimization problems can lead to tremendous speed-ups
- Very large number of shape design parameters are possible