

Mathematical details of adjoint-based shape optimization for the Euler and Reynolds-Averaged Navier-Stokes equations

(With thanks to Francisco Palacios, Jeff Fike, and Joaquim Martins)

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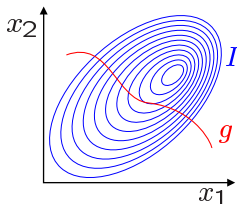
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OPTPDE 2011
July 5th, 2011 - Bilbao, Spain

Outline

- 1 Introduction
 - Optimal design in aerodynamics
 - Alternatives for sensitivity calculations
- 2 Design Using the Euler Equations
- 3 Design Using the RANS Equations
 - Spalart-Allmaras Turbulence Model
- 4 Continuous adjoint for the Spalart–Allmaras model
 - Analytical formulation
 - Transonic RAE-2822
 - Transonic NACA-0012
 - Optimization of a transonic airfoil
- 5 Conclusions

Introduction to Optimization



Non-linear program

minimize $I(\vec{x})$

$\vec{x} \in \mathbb{R}^{N_x}$

subject to $g_m(\vec{x}) \geq 0, \quad m = 1, 2, \dots, N_g$

- I : objective function, output (e.g. structural weight).
- x_n : vector of design variables, inputs (e.g. aerodynamic shape); bounds can be set on these variables.
- g_m : vector of constraints (e.g. element von Mises stresses); in general these are nonlinear functions of the design variables.

Optimization Methods



- **Intuition:** decreases with increasing dimensionality.
- **Grid or random search:** the cost of searching the design space increases rapidly with the number of design variables.
- **Evolutionary/Genetic algorithms:** good for discrete design variables and very robust; are they feasible when using a large number of design variables?
- **Nonlinear simplex:** simple and robust but inefficient for more than a few design variables.
- **Gradient-based:** the most efficient for a large number of design variables; assumes the objective function is “well-behaved”. Convergence only guaranteed to a local minimum.

Aerodynamic shape optimization

Shape optimization problem

Find $S^{\min} \in S_{\text{ad}}$ such that

$$J(S^{\min}) = \min_{S \in S_{\text{ad}}} J(S),$$

where $J(S) = \int_S j(U, \vec{n}, \vec{x}) ds$.

- Cost function j : drag/lift coefficients, deviation from pressure distribution, sonic boom intensity measures, total pressure loss, entropy increase. . .
- Surface parameterized by a suitable number of shape functions.

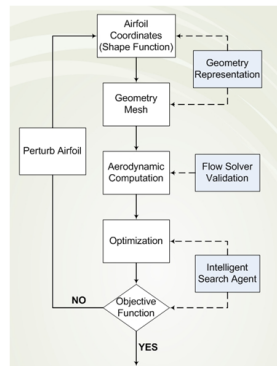
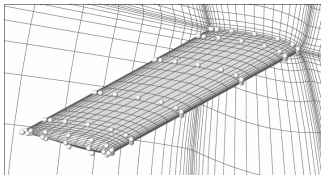
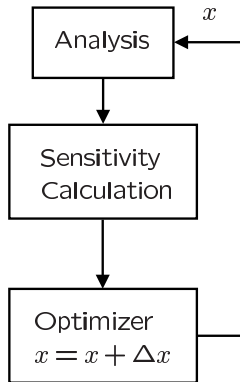


Figure 2: Flow diagram in aerodynamic optimization².

¹ J.E. Hicken, "Efficient algorithms for future aircraft design".

² M. Khurana, "Airfoil geometry parameterization through shape optimizer and computational fluid dynamics".

Gradient-Based Optimization: Design Cycle



- Analysis computes objective function and constraints (e.g. aero-structural solver)
- Optimizer uses the sensitivity information to search for the optimum solution (e.g. sequential quadratic programming)
- Sensitivity calculation is usually the bottleneck in the design cycle, particularly for large dimensional design spaces.
- Accuracy of the sensitivities is important, specially near the optimum.

Sensitivity Analysis Methods

- **Finite Differences:** very popular; easy, but lacks robustness and accuracy; run solver N_x times.

$$\frac{df}{dx_n} \approx \frac{f(x_n + h) - f(x)}{h} + \mathcal{O}(h)$$

- **Complex-Step Method:** relatively new; accurate and robust; easy to implement and maintain; run solver N_x times.

$$\frac{df}{dx_n} \approx \frac{\text{Im} [f(x_n + ih)]}{h} + \mathcal{O}(h^2)$$

- **Algorithmic/Automatic/Computational Differentiation:** accurate; ease of implementation and cost varies.
- **(Semi)-Analytic Methods:** efficient and accurate; long development time; **cost can be independent of N_x .**

Finite-Difference Derivative Approximations

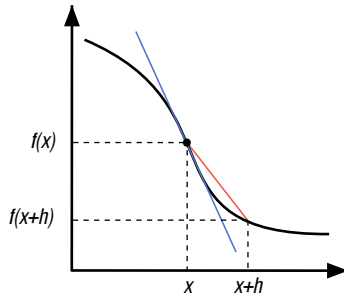
From Taylor series expansion,

$$f(x + h) = f(x) + hf'(x) + h^2 \frac{f''(x)}{2!} + h^3 \frac{f'''(x)}{3!} + \dots$$

Forward-difference approximation:

$$\Rightarrow \frac{df(x)}{dx} = \frac{f(x + h) - f(x)}{h} + \mathcal{O}(h).$$

$f(x)$	1,2345678901234 84
$f(x + h)$	1,234567890123456
Δf	0,0000000000000028



Complex-Step Derivative Approximation

Can also be derived from a Taylor series expansion about x with a complex step ih :

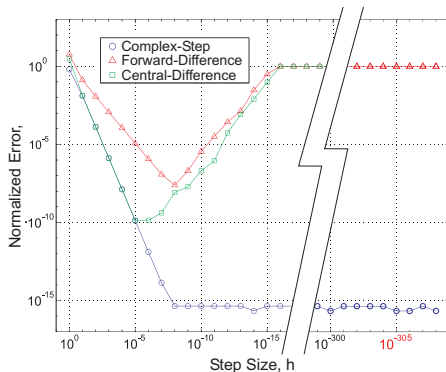
$$f(x + ih) = f(x) + ihf'(x) - h^2 \frac{f''(x)}{2!} - ih^3 \frac{f'''(x)}{3!} + \dots$$

$$\Rightarrow f'(x) = \frac{\operatorname{Im}[f(x + ih)]}{h} + h^2 \frac{f'''(x)}{3!} + \dots$$

$$\Rightarrow \boxed{f'(x) \approx \frac{\operatorname{Im}[f(x + ih)]}{h}}$$

No subtraction! Second order approximation. (Martins, Sturdza, Alonso, ACM Trans. Math. Soft., 2003)

Simple Numerical Example



Estimate derivative at $x = 1,5$ of the function,

$$f(x) = \frac{e^x}{\sqrt{\sin^3 x + \cos^3 x}}$$

Relative error defined as:

$$\epsilon = \frac{|f' - f'_{ref}|}{|f'_{ref}|}$$

Would You Like Second Derivatives?

Unfortunately, complex step formulations are also subject to subtractive cancellation when used for second derivatives? What can you do? If you are interested, we have recently developed a method based on *hyper-dual numbers* that gives exact second derivatives, independently of the step, h !

Hyper-dual numbers have one real part and three non-real parts:

$$X = X_0 + X_1\epsilon_1 + X_2\epsilon_2 + X_3\epsilon_1\epsilon_2$$

$$\epsilon_1^2 = \epsilon_2^2 = 0$$

$$\epsilon_1 \neq \epsilon_2 \neq 0$$

$$\epsilon_1\epsilon_2 = \epsilon_2\epsilon_1 \neq 0$$

With these definitions, the Taylor series expansion truncates *exactly* at the second-derivative term.

Hyper-Dual Numbers

In other words:

$$f(x + h_1\epsilon_1 + h_2\epsilon_2 + 0\epsilon_1\epsilon_2) = f(x) + h_1f'(x)\epsilon_1 + h_2f'(x)\epsilon_2 + h_1h_2f''(x)\epsilon_1\epsilon_2$$

There is no truncation error and no subtractive cancellation error (because of the definition of the hyper-dual numbers, see Fike and Alonso, AIAA-2011-3847). Evaluate a function with a hyper-dual step:

$$f(\vec{x} + h_1\epsilon_1\vec{e}_i + h_2\epsilon_2\vec{e}_j + \vec{0}\epsilon_1\epsilon_2)$$

Derivative information can be found by examining the non-real parts:

$$\frac{\partial f(\vec{x})}{\partial x_i} = \frac{\epsilon_1 \text{part}[f(\vec{x} + h_1\epsilon_1\vec{e}_i + h_2\epsilon_2\vec{e}_j + \vec{0}\epsilon_1\epsilon_2)]}{h_1}$$

$$\frac{\partial f(\vec{x})}{\partial x_j} = \frac{\epsilon_2 \text{part}[f(\vec{x} + h_1\epsilon_1\vec{e}_i + h_2\epsilon_2\vec{e}_j + \vec{0}\epsilon_1\epsilon_2)]}{h_2}$$

$$\frac{\partial^2 f(\vec{x})}{\partial x_i \partial x_j} = \frac{\epsilon_1 \epsilon_2 \text{part}[f(\vec{x} + h_1\epsilon_1\vec{e}_i + h_2\epsilon_2\vec{e}_j + \vec{0}\epsilon_1\epsilon_2)]}{h_1 h_2}$$

Challenges in Large-Scale Sensitivity Analysis

- There are efficient methods to obtain sensitivities of **many** functions with respect to a **few** design variables - **Direct Method**.
- There are efficient methods to obtain sensitivities of a **few** functions with respect to **many** design variables - **Adjoint method**.
- Unfortunately, there are **no** known methods to obtain sensitivities of **many** functions with respect to **many** design variables.
- This is the *curse of dimensionality*.

Symbolic Development of the Adjoint Method

Let I be the cost (or objective) function

$$I = I(\mathbf{w}, \mathcal{F})$$

where

\mathbf{w} = flow field variables

\mathcal{F} = grid variables

The first variation of the cost function is

$$\delta I = \frac{\partial I}{\partial \mathbf{w}}^T \delta \mathbf{w} + \frac{\partial I}{\partial \mathcal{F}}^T \delta \mathcal{F}$$

The flow field equation and its first variation are

$$R(\mathbf{w}, \mathcal{F}) = 0$$

$$\delta R = 0 = \left[\frac{\partial R}{\partial \mathbf{w}} \right] \delta \mathbf{w} + \left[\frac{\partial R}{\partial \mathcal{F}} \right] \delta \mathcal{F}$$

Symbolic Development of the Adjoint Method

Introducing a Lagrange Multiplier, ψ , and using the flow field equation as a constraint

$$\begin{aligned}\delta I &= \frac{\partial I}{\partial \mathbf{w}}^T \delta \mathbf{w} + \frac{\partial I}{\partial \mathcal{F}}^T \delta \mathcal{F} - \psi^T \left\{ \left[\frac{\partial \mathbf{R}}{\partial \mathbf{w}} \right] \delta \mathbf{w} + \left[\frac{\partial \mathbf{R}}{\partial \mathcal{F}} \right] \delta \mathcal{F} \right\} \\ &= \left\{ \frac{\partial I}{\partial \mathbf{w}}^T - \psi^T \left[\frac{\partial \mathbf{R}}{\partial \mathbf{w}} \right] \right\} \delta \mathbf{w} + \left\{ \frac{\partial I}{\partial \mathcal{F}}^T - \psi^T \left[\frac{\partial \mathbf{R}}{\partial \mathcal{F}} \right] \right\} \delta \mathcal{F}\end{aligned}$$

By choosing ψ such that it satisfies the adjoint equation

$$\left[\frac{\partial \mathbf{R}}{\partial \mathbf{w}} \right]^T \psi = \frac{\partial I}{\partial \mathbf{w}},$$

we have

$$\delta I = \left\{ \frac{\partial I}{\partial \mathcal{F}}^T - \psi^T \left[\frac{\partial \mathbf{R}}{\partial \mathcal{F}} \right] \right\} \delta \mathcal{F}$$

Symbolic Development of the Adjoint Method

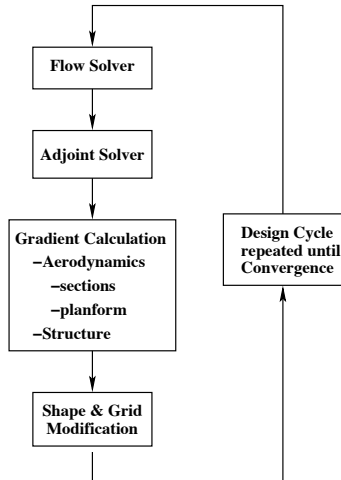
The expression for each component of the gradient no longer depends on δw and, therefore, no flow re-evaluation is needed (as is the case in finite-difference methods). Variations with respect to the shape $\delta \mathcal{F}$ can be computed with relatively little computational effort.

This reduces the gradient calculation for an arbitrarily large number of design variables at a single design point to

$$\begin{array}{c} \textbf{One Flow Solution} \\ + \\ \textbf{One Adjoint Solution} \end{array}$$

independently of the number of design parameters.

Design Cycle



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Design Using the Euler Equations

The following is a simplified version of the derivation of the adjoint equations and gradient computation formulae. In a body-fitted coordinate system, the Euler equations can be written in conservation law form as

$$\frac{\partial W}{\partial t} + \frac{\partial F_i}{\partial \xi_i} = 0 \quad \text{in } D, \quad (1)$$

where

$$W = Jw,$$

and

$$F_i = S_{ij}f_j.$$

The vector of conserved variables is typically given by:

$$w = \begin{pmatrix} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ \rho E \end{pmatrix} \quad f_j = \begin{pmatrix} \rho u_j \\ \rho u_1 u_j + p \delta_{1j} \\ \rho u_2 u_j + p \delta_{2j} \\ \rho u_3 u_j + p \delta_{3j} \\ \rho u_j H \end{pmatrix}$$

Design Using the Euler Equations

Assuming that the surface being designed, B_W , conforms to the computational plane $\xi_2 = 0$, the flow tangency condition can be written as

$$U_2 = 0 \quad \text{on } B_W. \quad (2)$$

Introduce the cost function

$$I = \frac{1}{2} \iint_{B_W} (p - p_d)^2 d\xi_1 d\xi_3.$$

A variation in the shape will cause a variation δp in the pressure and consequently a variation in the cost function

$$\delta I = \iint_{B_W} (p - p_d) \delta p d\xi_1 d\xi_3. \quad (3)$$

Since p depends on w through the equation of state the variation δp can be determined from the variation δw . Define the Jacobians

$$A_i = \frac{\partial f_i}{\partial w}, \quad C_i = S_{ij} A_j. \quad (4)$$

Formulation of the Design Problem

The weak form of the equation for δw in the steady state becomes

$$\int_{\mathcal{D}} \frac{\partial \psi^T}{\partial \xi_i} \delta F_i d\mathcal{D} = \int_{\mathcal{B}} (n_i \psi^T \delta F_i) d\mathcal{B},$$

where we have integrated the governing equations by parts and

$$\delta F_i = C_i \delta w + \delta S_{ij} f_j.$$

Adding to the variation of the cost function

$$\begin{aligned} \delta I = & \int \int_{B_W} (p - p_d) \delta p \, d\xi_1 d\xi_3 \\ & - \int_{\mathcal{D}} \left(\frac{\partial \psi^T}{\partial \xi_i} \delta F_i \right) d\mathcal{D} \\ & + \int_{\mathcal{B}} (n_i \psi^T \delta F_i) d\mathcal{B}, \end{aligned} \tag{5}$$

which should hold for an arbitrary choice of ψ .

Formulation of the Design Problem

In particular, the choice that satisfies the adjoint equation

$$\frac{\partial \psi}{\partial t} - C_i^T \frac{\partial \psi}{\partial \xi_i} = 0 \quad \text{in } D, \quad (6)$$

subject to far field boundary conditions

$$n_i \psi^T C_i \delta w = 0,$$

and solid wall conditions

$$S_{21}\psi_2 + S_{22}\psi_3 + S_{23}\psi_4 = (p - p_d) \quad \text{on } B_W, \quad (7)$$

yields and expression for the gradient that is *independent* of the variation in the flow solution δw :

$$\begin{aligned} \delta I &= - \int_D \frac{\partial \psi^T}{\partial \xi_i} \delta S_{ij} f_j d\mathcal{D} \\ &- \int \int_{B_W} (\delta S_{21}\psi_2 + \delta S_{22}\psi_3 + S_{23}\psi_4) p d\xi_1 d\xi_3. \end{aligned} \quad (8)$$

Formulation of the Design Problem

The volume integral in **blue** can be evaluated with ease (however, one needs to compute δS_{ij} using mesh perturbations). The surface integral in **red** is also easily evaluated. Note that there are other formulations where the volume integral can be converted to a surface integral (see next lecture) and the gradient evaluation is simplified considerably.

Why use the adjoint approach?

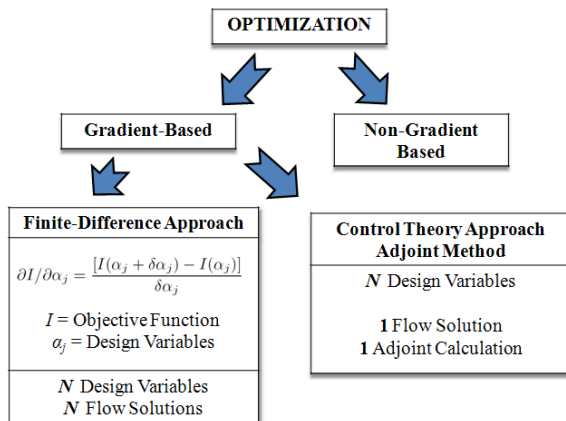


Figure 3: CFD as a design tool³.

³ P. Castonguay, S. Nadarajah, "Effect of shape parameterization on aerodynamic shape optimization".

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Viscous turbulent flows

- **Large Reynolds numbers:** the laminar motion becomes unstable and the fluid turns turbulent (most applications of industrial interest).

$350K < Re$



$200 < Re < 350K$



$40 < Re < 200$



$5 < Re < 40$



$Re < 5$

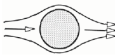


Figure 4: Flow transitions (experimental observations).

- **Turbulent flows** are computationally challenging because:
 - Fluid properties exhibit random spatial fluctuations.
 - Strong dependence from initial conditions.
 - Contain a wide range of scales (eddies).

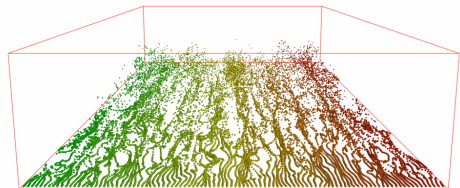


Figure 5: DNS simulation of a turbulent flow.

Reynolds Averaged Navier–Stokes equations

- Flow quantities are expressed as the sum of time fluctuations over small times scales about a steady or slowly varying mean flow:

$$u_i = \bar{u}_i + u'_i, \quad \rho = \bar{\rho} + \rho', \quad p = \bar{p} + p', \quad T = \bar{T} + T', \dots$$

- Averaging of the Navier–Stokes equations yields for the mean flow:

Navier–Stokes equations

- $\frac{\partial}{\partial t} \rho + \frac{\partial}{\partial x_j} (\rho u_j) = 0$
- $\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_j u_i) = -\frac{\partial}{\partial x_i} p + \frac{\partial}{\partial x_j} \tau_{ji}$
- $\frac{\partial}{\partial t} (\rho E) + \frac{\partial}{\partial x_j} (\rho u_j H) = \frac{\partial}{\partial x_j} (u_i \tau_{ij}) - \frac{\partial}{\partial x_j} q_j$

RANS equations

- $\frac{\partial}{\partial t} \bar{\rho} + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{u}_j) = 0$
- $\frac{\partial}{\partial t} (\bar{\rho} \bar{u}_i) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{u}_j \bar{u}_i) = -\frac{\partial}{\partial x_i} \bar{p} + \frac{\partial}{\partial x_j} \left[\bar{\tau}_{ji} - \overline{\rho u'_j u'_i} \right]$
- $\frac{\partial}{\partial t} (\bar{\rho} \bar{E}) + \frac{\partial}{\partial x_j} \left(\bar{\rho} \bar{u}_j \bar{H} + \frac{1}{2} \overline{\rho u'_j u'_j} \right) = \frac{\partial}{\partial x_j} \left[\bar{u}_i \left(\bar{\tau}_{ji} - \overline{\rho u'_j u'_i} \right) \right] - \frac{\partial}{\partial x_j} \left[\bar{q}_j + \overline{\rho u'_j H'} - \bar{\tau}_{ji} u'_i + \frac{1}{2} \overline{\rho u'_j u'_j u'_i} \right]$

- New terms require additional modeling to close the RANS equations.

Turbulent Spalart–Allmaras model

- The Spalart–Allmaras model solves an addition convection-diffusion equation (with a source term):

$$\begin{cases} \partial_t \hat{\nu} + \nabla \cdot \vec{T}^{cv} - T^s = 0 & \text{in } \Omega, \\ \hat{\nu} = 0 & \text{on } S, \\ \hat{\nu}_\infty = \sigma_\infty \nu_\infty & \text{on } \Gamma_\infty. \end{cases}$$

$$\vec{T}^{cv}(U, \hat{\nu}) = -\frac{\nu + \hat{\nu}}{\sigma} \nabla \hat{\nu} + \vec{\nu} \hat{\nu}$$

$$T^s(U, \hat{\nu}, d_S) = c_{b1} \hat{S} \hat{\nu} - c_{w1} f_w \left(\frac{\hat{\nu}}{d_S} \right)^2 + \frac{c_{b2}}{\sigma} |\nabla \hat{\nu}|^2$$

- Coupling to the main stream flow:

$$\mu_{tur} = \rho \hat{\nu} f_{v1} \quad \rightarrow \quad \mu_{tot}^1 = \mu_{dyn} + \mu_{tur} \quad \mu_{tot}^2 = \frac{\mu_{dyn}}{Pr_d} + \frac{\mu_{tur}}{Pr_t}$$

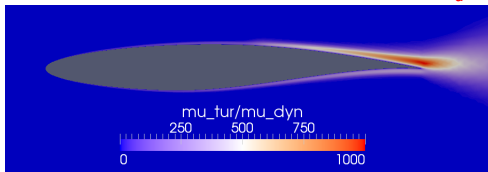


Figure 8: Ratio μ_{tur} / μ_{dyn} for a RAE-2822 profile in transonic conditions.

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Complete system of equations and boundary conditions

● **Navier–Stokes equations:**
$$\begin{cases} R_U(U, \hat{\nu}) = \nabla \cdot \vec{F}^c - \nabla \cdot (\mu_{tot}^1 \vec{F}^{\nu 1} + \mu_{tot}^2 \vec{F}^{\nu 2}) = 0 & \text{in } \Omega \\ \vec{\nu} = 0 & \text{on } S \\ \partial_n T = 0 & \text{on } S \\ (W)_+ = W_\infty & \text{on } \Gamma_\infty \end{cases}$$

$$\vec{F}_i^c = \begin{pmatrix} \rho v_i \\ \rho v_i v_1 + P \delta_{i1} \\ \rho v_i v_2 + P \delta_{i2} \\ \rho v_i v_3 + P \delta_{i3} \\ \rho v_i H \end{pmatrix}, \quad \vec{F}_i^{\nu 1} = \begin{pmatrix} \tau_{i1} \\ \tau_{i2} \\ \tau_{i3} \\ v_j \tau_{ij} \end{pmatrix}, \quad \vec{F}_i^{\nu 2} = \begin{pmatrix} \cdot \\ \cdot \\ \cdot \\ \cdot \\ C_p \partial_i T \end{pmatrix}, \quad i = 1, \dots, 3$$

$$\tau_{ij} = \partial_j v_i + \partial_i v_j - \frac{2}{3} \delta_{ij} \nabla \cdot \vec{\nu}, \quad \mu_{dyn} = \frac{\mu_1 T^{3/2}}{T + \mu_2}, \quad \mu_{tot}^1 = \mu_{dyn} + \mu_{tur}, \quad \mu_{tot}^2 = \frac{\mu_{dyn}}{Pr_d} + \frac{\mu_{tur}}{Pr_t}$$

● **Spalart–Allmaras model:**
$$\begin{cases} R_{\hat{\nu}}(U, \hat{\nu}, d_S) = \nabla \cdot \vec{T}^{CV} - T^S = 0 & \text{in } \Omega \\ \hat{\nu} = 0 & \text{on } S \\ \hat{\nu}_\infty = \sigma_\infty \nu_\infty & \text{on } \Gamma_\infty \end{cases}$$

$$\vec{T}^{CV}(U, \hat{\nu}) = -\frac{\nu + \hat{\nu}}{\sigma} \nabla \hat{\nu} + \hat{\nu} \nabla \hat{\nu}, \quad T^S(U, \hat{\nu}, d_S) = c_{b1} \hat{S} \hat{\nu} - c_{w1} f_w \left(\frac{\hat{\nu}}{d_S} \right)^2 + \frac{c_{b2}}{\sigma} |\nabla \hat{\nu}|^2.$$

$$\mu_{tur} = \rho \hat{\nu} f_{v1}, \quad f_{v1} = \frac{\chi^3}{\chi^3 + c_{v1}^3}, \quad \chi = \frac{\hat{\nu}}{\nu}, \quad \nu = \frac{\mu_{dyn}}{\rho}, \quad \hat{S} = |\hat{\Omega}| + \frac{\hat{\nu}}{\kappa^2 d_S^2} f_{v2}$$

$$f_{v2} = 1 - \frac{\chi}{1 + \chi f_{v1}}, \quad f_w = g \left[\frac{1 + c_{w3}^6}{g^6 + c_{w3}^6} \right]^{1/6}, \quad g = r + c_{w2}(r^6 - r), \quad r = \frac{\hat{\nu}}{\hat{S} \kappa^2 d_S^2}$$

● **Eikonal equation:**
$$\begin{cases} R_d(d_S) = |\nabla d_S|^2 - 1 = 0 & \text{in } \Omega \\ d_S = 0 & \text{on } S \end{cases}$$

Complete system of equations and boundary conditions

● **Navier–Stokes equations:**
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$$\tau_{ij} = \partial_j v_i + \partial_i v_j - \frac{2}{3} \delta_{ij} \nabla \cdot \vec{\nu}, \quad \mu_{dyn} = \frac{\mu_1 T^{3/2}}{T + \mu_2}, \quad \mu_{tot}^1 = \mu_{dyn} + \mu_{tur}, \quad \mu_{tot}^2 = \frac{\mu_{dyn}}{Pr_d} + \frac{\mu_{tur}}{Pr_t}$$

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$$\begin{cases} R_{\hat{\nu}}(U, \hat{\nu}, d_S) = \nabla \cdot \vec{T}^{CV} - T^S = 0 & \text{in } \Omega \\ \hat{\nu} = 0 & \text{on } S \\ \hat{\nu}_\infty = \sigma_\infty \nu_\infty & \text{on } \Gamma_\infty \end{cases}$$

$$\vec{T}^{CV}(U, \hat{\nu}) = -\frac{\nu + \hat{\nu}}{\sigma} \nabla \hat{\nu} + \vec{\nu} \hat{\nu}, \quad T^S(U, \hat{\nu}, d_S) = c_{b1} \hat{S} \hat{\nu} - c_{w1} f_w \left(\frac{\hat{\nu}}{d_S} \right)^2 + \frac{c_{b2}}{\sigma} |\nabla \hat{\nu}|^2.$$

$$\mu_{tur} = \rho \hat{\nu} f_{v1}, \quad f_{v1} = \frac{\chi^3}{\chi^3 + c_{v1}^3}, \quad \chi = \frac{\hat{\nu}}{\nu}, \quad \nu = \frac{\mu_{dyn}}{\rho}, \quad \hat{S} = |\hat{\Omega}| + \frac{\hat{\nu}}{\kappa^2 d_S^2} f_{v2}$$

$$f_{v2} = 1 - \frac{\chi}{1 + \chi f_{v1}}, \quad f_w = g \left[\frac{1 + c_{w3}^6}{g^6 + c_{w3}^6} \right]^{1/6}, \quad g = r + c_{w2}(r^6 - r), \quad r = \frac{\hat{\nu}}{\hat{S} \kappa^2 d_S^2}$$

● **Eikonal equation:**
$$\begin{cases} R_d(d_S) = |\nabla d_S|^2 - 1 = 0 & \text{in } \Omega \\ d_S = 0 & \text{on } S \end{cases}$$

Complete system of equations and boundary conditions

● **Navier–Stokes equations:**
$$\begin{cases} R_U(U, \hat{\nu}) = \nabla \cdot \vec{F}^C - \nabla \cdot (\mu_{tot}^1 \vec{F}^{v1} + \mu_{tot}^2 \vec{F}^{v2}) = 0 & \text{in } \Omega \\ \vec{\nu} = 0 & \text{on } S \\ \partial_n T = 0 & \text{on } S \\ (W)_+ = W_\infty & \text{on } \Gamma_\infty \end{cases}$$

$$\vec{F}_i^C = \begin{pmatrix} \rho v_i \\ \rho v_i v_1 + P \delta_{i1} \\ \rho v_i v_2 + P \delta_{i2} \\ \rho v_i v_3 + P \delta_{i3} \\ \rho v_i H \end{pmatrix}, \quad \vec{F}_i^{v1} = \begin{pmatrix} \tau_{i1} \\ \tau_{i2} \\ \tau_{i3} \\ v_j \tau_{ij} \end{pmatrix}, \quad \vec{F}_i^{v2} = \begin{pmatrix} \cdot \\ \cdot \\ \cdot \\ \cdot \\ C_p \partial_i T \end{pmatrix}, \quad i = 1, \dots, 3$$

$$\tau_{ij} = \partial_j v_i + \partial_i v_j - \frac{2}{3} \delta_{ij} \nabla \cdot \vec{\nu}, \quad \mu_{dyn} = \frac{\mu_1 T^{3/2}}{T + \mu_2}, \quad \mu_{tot}^1 = \mu_{dyn} + \mu_{tur}, \quad \mu_{tot}^2 = \frac{\mu_{dyn}}{Pr_d} + \frac{\mu_{tur}}{Pr_t}$$

● **Spalart–Allmaras model:**
$$\begin{cases} R_{\hat{\nu}}(U, \hat{\nu}, d_S) = \nabla \cdot \vec{T}^{CV} - T^S = 0 & \text{in } \Omega \\ \hat{\nu} = 0 & \text{on } S \\ \hat{\nu}_\infty = \sigma_\infty \nu_\infty & \text{on } \Gamma_\infty \end{cases}$$

$$\vec{T}^{CV}(U, \hat{\nu}) = -\frac{\nu + \hat{\nu}}{\sigma} \nabla \hat{\nu} + \vec{\nu} \hat{\nu}, \quad T^S(U, \hat{\nu}, d_S) = c_{b1} \hat{S} \hat{\nu} - c_{w1} f_w \left(\frac{\hat{\nu}}{d_S} \right)^2 + \frac{c_{b2}}{\sigma} |\nabla \hat{\nu}|^2.$$

$$\mu_{tur} = \rho \hat{\nu} f_{v1}, \quad f_{v1} = \frac{\chi^3}{\chi^3 + c_{v1}^3}, \quad \chi = \frac{\hat{\nu}}{\nu}, \quad \nu = \frac{\mu_{dyn}}{\rho}, \quad \hat{S} = |\hat{\Omega}| + \frac{\hat{\nu}}{\kappa^2 d_S^2} f_{v2}$$

$$f_{v2} = 1 - \frac{\chi}{1 + \chi f_{v1}}, \quad f_w = g \left[\frac{1 + c_{w3}^6}{g^6 + c_{w3}^6} \right]^{1/6}, \quad g = r + c_{w2}(r^6 - r), \quad r = \frac{\hat{\nu}}{\hat{S} \kappa^2 d_S^2}$$

● **Eikonal equation:**
$$\begin{cases} R_d(d_S) = |\nabla d_S|^2 - 1 = 0 & \text{in } \Omega \\ d_S = 0 & \text{on } S \end{cases}$$

Complete system of equations and boundary conditions

● **Navier–Stokes equations:**
$$\begin{cases} R_U(U, \hat{\nu}) = \nabla \cdot \vec{F}^C - \nabla \cdot (\mu_{tot}^1 \vec{F}^{\nu 1} + \mu_{tot}^2 \vec{F}^{\nu 2}) = 0 & \text{in } \Omega \\ \vec{\nu} = 0 & \text{on } S \\ \partial_n T = 0 & \text{on } S \\ (W)_+ = W_\infty & \text{on } \Gamma_\infty \end{cases}$$

$$\vec{F}_i^C = \begin{pmatrix} \rho v_i \\ \rho v_i v_1 + P \delta_{i1} \\ \rho v_i v_2 + P \delta_{i2} \\ \rho v_i v_3 + P \delta_{i3} \\ \rho v_i H \end{pmatrix}, \quad \vec{F}_i^{\nu 1} = \begin{pmatrix} \tau_{i1} \\ \tau_{i2} \\ \tau_{i3} \\ v_j \tau_{ij} \end{pmatrix}, \quad \vec{F}_i^{\nu 2} = \begin{pmatrix} \cdot \\ \cdot \\ \cdot \\ \cdot \\ C_p \partial_i T \end{pmatrix}, \quad i = 1, \dots, 3$$

$$\tau_{ij} = \partial_j v_i + \partial_i v_j - \frac{2}{3} \delta_{ij} \nabla \cdot \vec{\nu}, \quad \mu_{dyn} = \frac{\mu_1 T^{3/2}}{T + \mu_2}, \quad \mu_{tot}^1 = \mu_{dyn} + \mu_{tur}, \quad \mu_{tot}^2 = \frac{\mu_{dyn}}{Pr_d} + \frac{\mu_{tur}}{Pr_t}$$

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$$\begin{cases} R_{\hat{\nu}}(U, \hat{\nu}, d_S) = \nabla \cdot \vec{T}^{CV} - T^S = 0 & \text{in } \Omega \\ \hat{\nu} = 0 & \text{on } S \\ \hat{\nu}_\infty = \sigma_\infty \nu_\infty & \text{on } \Gamma_\infty \end{cases}$$

$$\vec{T}^{CV}(U, \hat{\nu}) = -\frac{\nu + \hat{\nu}}{\sigma} \nabla \hat{\nu} + \vec{\nu} \hat{\nu}, \quad T^S(U, \hat{\nu}, d_S) = c_{b1} \hat{S} \hat{\nu} - c_{w1} f_w \left(\frac{\hat{\nu}}{d_S} \right)^2 + \frac{c_{b2}}{\sigma} |\nabla \hat{\nu}|^2.$$

$$\mu_{tur} = \rho \hat{\nu} f_{v1}, \quad f_{v1} = \frac{\chi^3}{\chi^3 + c_{v1}^3}, \quad \chi = \frac{\hat{\nu}}{\nu}, \quad \nu = \frac{\mu_{dyn}}{\rho}, \quad \hat{S} = |\hat{\Omega}| + \frac{\hat{\nu}}{\kappa^2 d_S^2} f_{v2}$$

$$f_{v2} = 1 - \frac{\chi}{1 + \chi f_{v1}}, \quad f_w = g \left[\frac{1 + c_{w3}^6}{g^6 + c_{w3}^6} \right]^{1/6}, \quad g = r + c_{w2}(r^6 - r), \quad r = \frac{\hat{\nu}}{\hat{S} \kappa^2 d_S^2}$$

● **Eikonal equation:**
$$\begin{cases} R_d(d_S) = |\nabla d_S|^2 - 1 = 0 & \text{in } \Omega \\ d_S = 0 & \text{on } S \end{cases}$$

Objective function and surface deformation

- We consider the following choice of objective function:

$$J(S) = \int_S j(\vec{f}, T, \partial_n \hat{v}, \vec{n}) ds, \quad \vec{f} = P\vec{n} - \vec{\sigma} \cdot \vec{n}.$$

- Incorporating flow equations as constraints to the cost functional by means of Lagrange multipliers, the Lagrangian reads:

$$\begin{aligned} \mathcal{J}(S) = & \int_S j(\vec{f}, T, \partial_n \hat{v}, \vec{n}) ds \\ & + \int_{\Omega} \left(\Psi_U^T R_U(U, \hat{v}) + \psi_{\hat{v}} R_{\hat{v}}(U, \hat{v}, d_S) + \psi_d R_d(d_S) \right) dx. \end{aligned}$$

- We consider deformations of size δS along the normal direction to the surface $S' = \{\vec{x} + \delta S \vec{n}, \vec{x} \in S\}$. So, the following holds:

$$\begin{cases} \delta \vec{n} = -\nabla_S(\delta S) \\ \delta(ds) = -2H_m \delta S ds \end{cases}$$

Variation of the functional under the deformation

Total variation of the functional

$$\begin{aligned}\delta \mathcal{J} = & \int_S \delta j(\vec{f}, T, \partial_n \hat{v}, \vec{n}) ds + \int_{\delta S} j(\vec{f}, T, \partial_n \hat{v}, \vec{n}) ds \\ & + \int_{\Omega} \left(\Psi_U^T \delta R_U(U, \hat{v}) + \psi_{\hat{v}} \delta R_{\hat{v}}(U, \hat{v}, d_S) + \psi_d \delta R_d(d_S) \right) dx\end{aligned}$$

- Linearization of the system of equations:

$$\begin{aligned}\text{N.S.: } & \begin{cases} \frac{\partial R_U}{\partial U} \delta U = \nabla \cdot (\vec{A}^c \delta U) - \nabla \cdot \left(\vec{F}^{vk} \frac{\partial \mu_{tot}^k}{\partial U} \delta U + \mu_{tot}^k \vec{A}^{vk} \delta U + \mu_{tot}^k \mathbf{D}^{vk} \nabla \delta U \right) \\ \frac{\partial R_U}{\partial \hat{v}} \delta \hat{v} = -\nabla \cdot \left(\vec{F}^{vk} \frac{\partial \mu_{tot}^k}{\partial \hat{v}} \delta \hat{v} \right) \end{cases} \\ \text{S.A.: } & \begin{cases} \frac{\partial R_U}{\partial U} \delta U = \nabla \cdot (\vec{F}^{cv} \delta U) - F^s \delta U - \mathbf{M}^s \nabla \delta U \\ \frac{\partial R_{\hat{v}}}{\partial \hat{v}} \delta \hat{v} = \nabla \cdot (\vec{B}^{cv} \delta \hat{v} + \mathbf{E}^{cv} \nabla \delta \hat{v}) - B^s \delta \hat{v} - \mathbf{E}^s \nabla \delta \hat{v} \\ \frac{\partial R_{\hat{v}}}{\partial d_S} \delta d_S = -K^s \delta d_S \end{cases} \\ \text{Eikonal: } & \begin{cases} \frac{\partial R_d}{\partial d_S} \delta d_S = \nabla d_S \cdot \nabla \delta d_S = 0 \end{cases}\end{aligned}$$

Variation of the functional under the deformation

Total variation of the functional

$$\begin{aligned} \delta \mathcal{J} = & \int_S \delta j(\vec{f}, T, \partial_n \hat{v}, \vec{n}) ds + \int_{\delta S} j(\vec{f}, T, \partial_n \hat{v}, \vec{n}) ds \\ & + \int_{\Omega} \left(\Psi_U^T \delta R_U(U, \hat{v}) + \psi_{\hat{v}} \delta R_{\hat{v}}(U, \hat{v}, d_S) + \psi_d \delta R_d(d_S) \right) dx \end{aligned}$$

- Linearization of the system of equations:

$$\begin{aligned} \text{N.S.:} & \begin{cases} \frac{\partial R_U}{\partial U} \delta U = \nabla(\vec{A}^c \delta U) - \nabla \cdot \left(\vec{F}^{vk} \frac{\partial \mu_{tot}^k}{\partial U} \delta U + \mu_{tot}^k \vec{A}^{vk} \delta U + \mu_{tot}^k \mathbf{D}^{vk} \nabla \delta U \right) \\ \frac{\partial R_{\hat{v}}}{\partial \hat{v}} \delta \hat{v} = -\nabla \cdot \left(\vec{F}^{vk} \frac{\partial \mu_{tot}^k}{\partial \hat{v}} \delta \hat{v} \right) \end{cases} \\ \text{S.A.:} & \begin{cases} \frac{\partial R_U}{\partial U} \delta U = \nabla \cdot (\vec{F}^{cv} \delta U) - F^s \delta U - \mathbf{M}^s \nabla \delta U \\ \frac{\partial R_{\hat{v}}}{\partial \hat{v}} \delta \hat{v} = \nabla \cdot (\vec{B}^{cv} \delta \hat{v} + \mathbf{E}^{cv} \nabla \delta \hat{v}) - B^s \delta \hat{v} - \mathbf{E}^s \nabla \delta \hat{v} \\ \frac{\partial R_d}{\partial d_S} \delta d_S = -K^s \delta d_S \end{cases} \\ \text{Eikonal:} & \begin{cases} \frac{\partial R_d}{\partial d_S} \delta d_S = \nabla d_S \cdot \nabla \delta d_S = 0 \end{cases} \end{aligned}$$

Variation of the functional under the deformation

Total variation of the functional

$$\begin{aligned} \delta \mathcal{J} = & \int_S \delta j(\vec{f}, T, \partial_n \hat{v}, \vec{n}) ds + \int_{\delta S} j(\vec{f}, T, \partial_n \hat{v}, \vec{n}) ds \\ & + \int_{\Omega} \left(\Psi_U^T \delta R_U(U, \hat{v}) + \psi_{\hat{v}} \delta R_{\hat{v}}(U, \hat{v}, d_S) + \psi_d \delta R_d(d_S) \right) dx \end{aligned}$$

- Linearization of the system of equations:

$$\begin{aligned} \text{N.S.:} & \begin{cases} \frac{\partial R_U}{\partial U} \delta U = \nabla \cdot (\vec{A}^c \delta U) - \nabla \cdot \left(\vec{F}^{vk} \frac{\partial \mu_{tot}^k}{\partial U} \delta U + \mu_{tot}^k \vec{A}^{vk} \delta U + \mu_{tot}^k \mathbf{D}^{vk} \nabla \delta U \right) \\ \frac{\partial R_U}{\partial \hat{v}} \delta \hat{v} = -\nabla \cdot \left(\vec{F}^{vk} \frac{\partial \mu_{tot}^k}{\partial \hat{v}} \delta \hat{v} \right) \end{cases} \\ \text{S.A.:} & \begin{cases} \frac{\partial R_U}{\partial U} \delta U = \nabla \cdot (\vec{F}^{cv} \delta U) - F^s \delta U - \mathbf{M}^s \nabla \delta U \\ \frac{\partial R_{\hat{v}}}{\partial \hat{v}} \delta \hat{v} = \nabla \cdot \left(\vec{B}^{cv} \delta \hat{v} + \mathbf{E}^{cv} \nabla \delta \hat{v} \right) - B^s \delta \hat{v} - \mathbf{E}^s \nabla \delta \hat{v} \\ \frac{\partial R_{\hat{v}}}{\partial d_S} \delta d_S = -K^s \delta d_S \end{cases} \\ \text{Eikonal:} & \begin{cases} \frac{\partial R_d}{\partial d_S} \delta d_S = \nabla d_S \cdot \nabla \delta d_S = 0 \end{cases} \end{aligned}$$

Complete continuous adjoint method

System of adjoint equations

$$\left\{ \begin{array}{l} 0 = A_U^U \Psi_U + A_{\hat{v}}^U \psi_{\hat{v}} \\ 0 = A_U^{\hat{v}} \Psi_U + A_{\hat{v}}^{\hat{v}} \psi_{\hat{v}} \\ 0 = A_d^{\hat{v}} \psi_{\hat{v}} + A_d^d \psi_d \end{array} \right. \quad BCs : \left\{ \begin{array}{l} \varphi_i = -\frac{\partial j}{\partial f_i} - \psi_{\hat{v}} g_4 n_i \\ \partial n \psi_5 = -\frac{1}{g_2} \left(\frac{\partial j}{\partial T} - \vec{g}_1 \cdot \vec{\varphi} + \psi_{\hat{v}} g_5 \right) \\ \psi_{\hat{v}} = -\frac{1}{g_3} \frac{\partial j}{\partial (\partial_n \hat{v})} \\ \psi_d = 0 \end{array} \right.$$

● Adjoint operators:

$$A_U^U \Psi_U = -\nabla \Psi_U^T \cdot \vec{A}^c - \nabla \cdot \left(\nabla \Psi_U^T \cdot \mu_{tot}^k \mathbf{D}^{vk} \right) + \nabla \Psi_U^T \cdot \mu_{tot}^k \vec{A}^{vk} + \nabla \Psi_U^T \cdot \vec{F}^{vk} \frac{\partial \mu_{tot}^k}{\partial U}$$

$$A_{\hat{v}}^U \psi_{\hat{v}} = -\nabla \psi_{\hat{v}} \cdot \vec{F}^{cv} - \psi_{\hat{v}} F^s + \nabla \cdot (\psi_{\hat{v}} \mathbf{M}^s)$$

$$A_U^{\hat{v}} \Psi_U = \nabla \Psi_U^T \cdot \vec{F}^{vk} \frac{\partial \mu_{tot}^k}{\partial \hat{v}}$$

$$A_{\hat{v}}^{\hat{v}} \psi_{\hat{v}} = -\nabla \psi_{\hat{v}} \cdot \vec{B}^{cv} + \nabla \cdot (\nabla \psi_{\hat{v}} \cdot \mathbf{E}^{cv}) - \psi_{\hat{v}} B^s + \nabla \cdot (\psi_{\hat{v}} \mathbf{E}^s)$$

$$A_{\hat{v}}^d \psi_{\hat{v}} = -K^s \psi_{\hat{v}}$$

$$A_d^d \psi_d = -\nabla \cdot (\psi_d \nabla d_s)$$

Complete continuous adjoint method

System of adjoint equations

$$\left\{ \begin{array}{l} 0 = A_U^U \Psi_U + A_{\hat{v}}^U \psi_{\hat{v}} \\ 0 = A_U^{\hat{v}} \Psi_U + A_{\hat{v}}^{\hat{v}} \psi_{\hat{v}} \\ 0 = A_{\hat{v}}^d \psi_{\hat{v}} + A_d^d \psi_d \end{array} \right. \quad BCs : \left\{ \begin{array}{l} \varphi_i = -\frac{\partial j}{\partial f_i} - \psi_{\hat{v}} g_4 n_i \\ \partial n \psi_5 = -\frac{1}{g_2} \left(\frac{\partial j}{\partial T} - \vec{g}_1 \cdot \vec{\varphi} + \psi_{\hat{v}} g_5 \right) \\ \psi_{\hat{v}} = -\frac{1}{g_3} \frac{\partial j}{\partial (\partial_n \hat{v})} \\ \psi_d = 0 \end{array} \right.$$

● Adjoint operators:

$$A_U^U \Psi_U = -\nabla \Psi_U^T \cdot \vec{A}^c - \nabla \cdot \left(\nabla \Psi_U^T \cdot \mu_{tot}^k \mathbf{D}^{vk} \right) + \nabla \Psi_U^T \cdot \mu_{tot}^k \vec{A}^{vk} + \nabla \Psi_U^T \cdot \vec{F}^{vk} \frac{\partial \mu_{tot}^k}{\partial U}$$

$$A_{\hat{v}}^U \psi_{\hat{v}} = -\nabla \psi_{\hat{v}} \cdot \vec{F}^{cv} - \psi_{\hat{v}} F^s + \nabla \cdot (\psi_{\hat{v}} \mathbf{M}^s)$$

$$A_U^{\hat{v}} \Psi_U = \nabla \Psi_U^T \cdot \vec{F}^{vk} \frac{\partial \mu_{tot}^k}{\partial \hat{v}}$$

$$A_{\hat{v}}^{\hat{v}} \psi_{\hat{v}} = -\nabla \psi_{\hat{v}} \cdot \vec{B}^{cv} + \nabla \cdot (\nabla \psi_{\hat{v}} \cdot \mathbf{E}^{cv}) - \psi_{\hat{v}} B^s + \nabla \cdot (\psi_{\hat{v}} \mathbf{E}^s)$$

$$A_{\hat{v}}^d \psi_{\hat{v}} = -K^s \psi_{\hat{v}}$$

$$A_d^d \psi_d = -\nabla \cdot (\psi_d \nabla d_s)$$

Complete continuous adjoint method

System of adjoint equations

$$\left\{ \begin{array}{l} 0 = A_U^U \psi_U + A_{\hat{v}}^U \psi_{\hat{v}} \\ 0 = A_U^{\hat{v}} \psi_U + A_{\hat{v}}^{\hat{v}} \psi_{\hat{v}} \\ 0 = A_d^d \psi_{\hat{v}} + A_d^d \psi_d \end{array} \right. \quad BCs : \left\{ \begin{array}{l} \varphi_i = -\frac{\partial j}{\partial f_i} - \psi_{\hat{v}} g_4 n_i \\ \partial n \psi_5 = -\frac{1}{g_2} \left(\frac{\partial j}{\partial T} - \vec{g}_1 \cdot \vec{\varphi} + \psi_{\hat{v}} g_5 \right) \\ \psi_{\hat{v}} = -\frac{1}{g_3} \frac{\partial j}{\partial (\partial_n \hat{v})} \\ \psi_d = 0 \end{array} \right.$$

● Adjoint operators:

$$A_U^U \psi_U = -\nabla \Psi_U^T \cdot \vec{A}^c - \nabla \cdot \left(\nabla \Psi_U^T \cdot \mu_{tot}^k \mathbf{D}^{vk} \right) + \nabla \Psi_U^T \cdot \mu_{tot}^k \vec{A}^{vk} + \nabla \Psi_U^T \cdot \vec{F}^{vk} \frac{\partial \mu_{tot}^k}{\partial U}$$

$$A_U^{\hat{v}} \psi_{\hat{v}} = -\nabla \psi_{\hat{v}} \cdot \vec{F}^{cv} - \psi_{\hat{v}} F^s + \nabla \cdot (\psi_{\hat{v}} \mathbf{M}^s)$$

$$A_U^{\hat{v}} \psi_U = \nabla \Psi_U^T \cdot \vec{F}^{vk} \frac{\partial \mu_{tot}^k}{\partial \hat{v}}$$

$$A_{\hat{v}}^{\hat{v}} \psi_{\hat{v}} = -\nabla \psi_{\hat{v}} \cdot \vec{B}^{cv} + \nabla \cdot (\nabla \psi_{\hat{v}} \cdot \mathbf{E}^{cv}) - \psi_{\hat{v}} B^s + \nabla \cdot (\psi_{\hat{v}} \mathbf{E}^s)$$

$$A_{\hat{v}}^d \psi_{\hat{v}} = -K^s \psi_{\hat{v}}$$

$$A_d^d \psi_d = -\nabla \cdot (\psi_d \nabla d_s)$$

Complete continuous adjoint method

System of adjoint equations

$$\left\{ \begin{array}{l} 0 = A_U^U \psi_U + A_{\hat{v}}^U \psi_{\hat{v}} \\ 0 = A_U^{\hat{v}} \psi_U + A_{\hat{v}}^{\hat{v}} \psi_{\hat{v}} \\ 0 = A_d^d \psi_{\hat{v}} + A_d^d \psi_d \end{array} \right. \quad BCs : \left\{ \begin{array}{l} \varphi_i = -\frac{\partial j}{\partial f_i} - \psi_{\hat{v}} g_4 n_i \\ \partial n \psi_5 = -\frac{1}{g_2} \left(\frac{\partial j}{\partial T} - \vec{g}_1 \cdot \vec{\varphi} + \psi_{\hat{v}} g_5 \right) \\ \psi_{\hat{v}} = -\frac{1}{g_3} \frac{\partial j}{\partial (\partial_n \hat{v})} \\ \psi_d = 0 \end{array} \right.$$

● Adjoint operators:

$$A_U^U \psi_U = -\nabla \Psi_U^T \cdot \vec{A}^c - \nabla \cdot \left(\nabla \Psi_U^T \cdot \mu_{tot}^k \mathbf{D}^{vk} \right) + \nabla \Psi_U^T \cdot \mu_{tot}^k \vec{A}^{vk} + \nabla \Psi_U^T \cdot \vec{F}^{vk} \frac{\partial \mu_{tot}^k}{\partial U}$$

$$A_U^{\hat{v}} \psi_{\hat{v}} = -\nabla \psi_{\hat{v}} \cdot \vec{F}^{cv} - \psi_{\hat{v}} F^s + \nabla \cdot (\psi_{\hat{v}} \mathbf{M}^s)$$

$$A_U^{\hat{v}} \psi_U = \nabla \Psi_U^T \cdot \vec{F}^{vk} \frac{\partial \mu_{tot}^k}{\partial \hat{v}}$$

$$A_{\hat{v}}^{\hat{v}} \psi_{\hat{v}} = -\nabla \psi_{\hat{v}} \cdot \vec{B}^{cv} + \nabla \cdot (\nabla \psi_{\hat{v}} \cdot \mathbf{E}^{cv}) - \psi_{\hat{v}} B^s + \nabla \cdot (\psi_{\hat{v}} \mathbf{E}^s)$$

$$A_{\hat{v}}^d \psi_{\hat{v}} = -K^s \psi_{\hat{v}}$$

$$A_d^d \psi_d = -\nabla \cdot (\psi_d \nabla d_s)$$

Complete continuous adjoint method

System of adjoint equations

$$\left\{ \begin{array}{l} 0 = A_U^U \psi_U + A_{\hat{v}}^U \psi_{\hat{v}} \\ 0 = A_U^{\hat{v}} \psi_U + A_{\hat{v}}^{\hat{v}} \psi_{\hat{v}} \\ 0 = A_d^d \psi_d + A_d^{\hat{v}} \psi_{\hat{v}} \end{array} \right. \quad BCs : \left\{ \begin{array}{l} \varphi_i = -\frac{\partial j}{\partial f_i} - \psi_{\hat{v}} g_4 n_i \\ \partial n \psi_5 = -\frac{1}{g_2} \left(\frac{\partial j}{\partial T} - \vec{g}_1 \cdot \vec{\varphi} + \psi_{\hat{v}} g_5 \right) \\ \psi_{\hat{v}} = -\frac{1}{g_3} \frac{\partial j}{\partial (\partial_n \hat{v})} \\ \psi_d = 0 \end{array} \right.$$

● Adjoint operators:

$$A_U^U \psi_U = -\nabla \Psi_U^T \cdot \vec{A}^c - \nabla \cdot \left(\nabla \Psi_U^T \cdot \mu_{tot}^k \mathbf{D}^{vk} \right) + \nabla \Psi_U^T \cdot \mu_{tot}^k \vec{A}^{vk} + \nabla \Psi_U^T \cdot \vec{F}^{vk} \frac{\partial \mu_{tot}^k}{\partial U}$$

$$A_U^{\hat{v}} \psi_{\hat{v}} = -\nabla \psi_{\hat{v}} \cdot \vec{F}^{cv} - \psi_{\hat{v}} F^s + \nabla \cdot (\psi_{\hat{v}} \mathbf{M}^s)$$

$$A_U^{\hat{v}} \psi_U = \nabla \Psi_U^T \cdot \vec{F}^{vk} \frac{\partial \mu_{tot}^k}{\partial \hat{v}}$$

$$A_{\hat{v}}^{\hat{v}} \psi_{\hat{v}} = -\nabla \psi_{\hat{v}} \cdot \vec{B}^{cv} + \nabla \cdot (\nabla \psi_{\hat{v}} \cdot \mathbf{E}^{cv}) - \psi_{\hat{v}} B^s + \nabla \cdot (\psi_{\hat{v}} \mathbf{E}^s)$$

$$A_{\hat{v}}^d \psi_{\hat{v}} = -K^s \psi_{\hat{v}}$$

$$A_d^d \psi_d = -\nabla \cdot (\psi_d \nabla d_s)$$

Complete adjoint vs. Frozen viscosity

System of adjoint equations

$$\begin{cases} 0 = A_U^U \Psi_U + A_{\hat{\nu}}^U \psi_{\hat{\nu}} \\ 0 = A_U^{\hat{\nu}} \Psi_U + A_{\hat{\nu}}^{\hat{\nu}} \psi_{\hat{\nu}} \end{cases} \quad BCs : \begin{cases} \varphi_i = -\frac{\partial j}{\partial f_i} - \psi_{\hat{\nu}} g_4 n_i \\ \partial n \psi_5 = -\frac{1}{g_2} \left(\frac{\partial j}{\partial T} - \vec{g}_1 \cdot \vec{\varphi} \right) - \frac{g_5}{g_2} \psi_{\hat{\nu}} \\ \psi_{\hat{\nu}} = -\frac{1}{g_3} \frac{\partial j}{\partial (\partial n \hat{\nu})} \end{cases}$$

Adjoint operators:

$$A_U^U \Psi_U = -\nabla \Psi_U^T \cdot \bar{A}^c - \nabla \cdot \left(\nabla \Psi_U^T \cdot \mu_{tot}^k \mathbf{D}^{vk} \right) + \nabla \Psi_U^T \cdot \mu_{tot}^k \bar{A}^{vk} + \nabla \Psi_U^T \cdot \bar{F}^{vk} \frac{\partial \mu_{tot}^k}{\partial U}$$

$$A_{\hat{\nu}}^U \psi_{\hat{\nu}} = -\nabla \psi_{\hat{\nu}} \cdot \bar{F}^{cv} - \psi_{\hat{\nu}} F^s + \nabla \cdot (\psi_{\hat{\nu}} \mathbf{M}^s)$$

$$A_U^{\hat{\nu}} \Psi_U = \nabla \Psi_U^T \cdot \bar{F}^{vk} \frac{\partial \mu_{tot}^k}{\partial \hat{\nu}}$$

$$A_{\hat{\nu}}^{\hat{\nu}} \psi_{\hat{\nu}} = -\nabla \psi_{\hat{\nu}} \cdot \bar{B}^{cv} + \nabla \cdot (\nabla \psi_{\hat{\nu}} \cdot \mathbf{E}^{cv}) - \psi_{\hat{\nu}} B^s + \nabla \cdot (\psi_{\hat{\nu}} \mathbf{E}^s)$$

Complete adjoint vs. Frozen viscosity

System of adjoint equations

$$\begin{cases} 0 = A_U^U \Psi_U + A_{\hat{\nu}}^U \psi_{\hat{\nu}} \\ 0 = A_U^{\hat{\nu}} \Psi_U + A_{\hat{\nu}}^{\hat{\nu}} \psi_{\hat{\nu}} \end{cases} \quad BCs : \begin{cases} \varphi_i = -\frac{\partial j}{\partial f_i} - \psi_{\hat{\nu}} g_4 n_i \\ \partial n \psi_5 = -\frac{1}{g_2} \left(\frac{\partial j}{\partial T} - \vec{g}_1 \cdot \vec{\varphi} \right) - \frac{g_5}{g_2} \psi_{\hat{\nu}} \\ \psi_{\hat{\nu}} = -\frac{1}{g_3} \frac{\partial j}{\partial (\partial n \hat{\nu})} \end{cases}$$

Adjoint operators:

$$A_U^U \Psi_U = -\nabla \Psi_U^T \cdot \vec{A}^c - \nabla \cdot \left(\nabla \Psi_U^T \cdot \mu_{tot}^k \mathbf{D}^{vk} \right) + \nabla \Psi_U^T \cdot \mu_{tot}^k \vec{A}^{vk} + \nabla \Psi_U^T \cdot \vec{F}^{vk} \frac{\partial \mu_{tot}^k}{\partial U}$$

$$A_{\hat{\nu}}^U \psi_{\hat{\nu}} = -\nabla \psi_{\hat{\nu}} \cdot \vec{F}^{cv} - \psi_{\hat{\nu}} F^s + \nabla \cdot (\psi_{\hat{\nu}} \mathbf{M}^s)$$

$$A_U^{\hat{\nu}} \Psi_U = \nabla \Psi_U^T \cdot \vec{F}^{vk} \frac{\partial \mu_{tot}^k}{\partial \hat{\nu}}$$

$$A_{\hat{\nu}}^{\hat{\nu}} \psi_{\hat{\nu}} = -\nabla \psi_{\hat{\nu}} \cdot \vec{B}^{cv} + \nabla \cdot (\nabla \psi_{\hat{\nu}} \cdot \mathbf{E}^{cv}) - \psi_{\hat{\nu}} B^s + \nabla \cdot (\psi_{\hat{\nu}} \mathbf{E}^s)$$

Evaluation of surface sensitivities

- Solving the adjoint system and introducing in the variation of the functional:

$$\begin{aligned}\delta \mathcal{J} = & \int_S \left(\frac{\partial j}{\partial f_i} \partial_n f_i + \frac{\partial j}{\partial T} \partial_n T + \frac{\partial j}{\partial (\partial_n \hat{v})} \partial_n^2 \hat{v} \right) \delta S \, ds \\ & - \int_S \left(\frac{\partial j}{\partial \vec{n}} + \frac{\partial j}{\partial \vec{f}} P - \frac{\partial j}{\partial \vec{f}} \cdot \vec{\sigma} \right) \cdot \nabla_S (\delta S) \, ds - \int_S (\hat{g} + 2H_m j) \delta S \, ds \\ & - 2 \int_S \psi_{\hat{v}} g_4 (P \vec{n} - \vec{n} \cdot \vec{\sigma}) \cdot \nabla_S (\delta S) \, ds.\end{aligned}$$

- Usual objective functions are of the form $j(\vec{f}) = \vec{f} \cdot \vec{d}$. Then:

Sensitivity computation

$$\delta \mathcal{J} = - \int_S h_3 \delta S \, ds$$

where

$$\begin{aligned}h_3 = & -\vec{n} \cdot \vec{\Sigma}^\varphi \cdot \partial_n \vec{v} + \mu_{tot}^2 C_p \nabla_S \psi_5 \cdot \nabla_S T \\ \vec{\Sigma}^\varphi = & \mu_{tot}^1 \left(\nabla \varphi + \nabla \varphi^T - \mathbf{I}_d \frac{2}{3} \nabla \cdot \varphi \right)\end{aligned}$$

Evaluation of surface sensitivities

- Solving the adjoint system and introducing in the variation of the functional:

$$\begin{aligned}\delta \mathcal{J} = & \int_S \left(\frac{\partial j}{\partial f_i} \partial_n f_i + \frac{\partial j}{\partial T} \partial_n T + \frac{\partial j}{\partial (\partial_n \hat{v})} \partial_n^2 \hat{v} \right) \delta S \, ds \\ & - \int_S \left(\frac{\partial j}{\partial \vec{n}} + \frac{\partial j}{\partial \vec{f}} P - \frac{\partial j}{\partial \vec{f}} \cdot \vec{\sigma} \right) \cdot \nabla_S (\delta S) \, ds - \int_S (\hat{g} + 2H_m j) \delta S \, ds \\ & - 2 \int_S \psi_{\hat{v}} g_4 (P \vec{n} - \vec{n} \cdot \vec{\sigma}) \cdot \nabla_S (\delta S) \, ds.\end{aligned}$$

- Usual objective functions are of the form $j(\vec{f}) = \vec{f} \cdot \vec{d}$. Then:

Sensitivity computation

$$\delta \mathcal{J} = - \int_S h_3 \delta S \, ds$$

where

$$\begin{aligned}h_3 &= -\vec{n} \cdot \bar{\Sigma}^\varphi \cdot \partial_n \vec{v} + \mu_{tot}^2 C_p \nabla_S \psi_5 \cdot \nabla_S T \\ \bar{\Sigma}^\varphi &= \mu_{tot}^1 \left(\nabla \vec{\varphi} + \nabla \vec{\varphi}^T - \mathbf{I}_d \frac{2}{3} \nabla \cdot \vec{\varphi} \right)\end{aligned}$$

Evaluation of surface sensitivities

- Solving the adjoint system and introducing in the variation of the functional:

$$\begin{aligned}\delta \mathcal{J} = & \int_S \left(\frac{\partial j}{\partial f_i} \partial_n f_i + \frac{\partial j}{\partial T} \partial_n T + \frac{\partial j}{\partial (\partial_n \hat{v})} \partial_n^2 \hat{v} \right) \delta S \, ds \\ & - \int_S \left(\frac{\partial j}{\partial \vec{n}} + \frac{\partial j}{\partial \vec{f}} P - \frac{\partial j}{\partial \vec{f}} \cdot \vec{\sigma} \right) \cdot \nabla_S (\delta S) \, ds - \int_S (\hat{g} + 2H_m j) \delta S \, ds \\ & - 2 \int_S \psi_{\hat{v}} g_4 (P \vec{n} - \vec{n} \cdot \vec{\sigma}) \cdot \nabla_S (\delta S) \, ds.\end{aligned}$$

- Usual objective functions are of the form $j(\vec{f}) = \vec{f} \cdot \vec{d}$. Then:

Sensitivity computation

$$\delta \mathcal{J} = - \int_S h_3 \delta S \, ds$$

where

$$\begin{aligned}h_3 &= -\vec{n} \cdot \bar{\Sigma}^\varphi \cdot \partial_n \vec{v} + \mu_{tot}^2 C_p \nabla_S \psi_5 \cdot \nabla_S T \\ \bar{\Sigma}^\varphi &= \mu_{tot}^1 \left(\nabla \vec{\varphi} + \nabla \vec{\varphi}^T - \mathbf{I}_d \frac{2}{3} \nabla \cdot \vec{\varphi} \right)\end{aligned}$$

Numerical experiments

- Transonic RAE-2822
($M_\infty = 0,734$; $Re = 6,5 \times 10^6$; $\alpha = 2,54^\circ$)

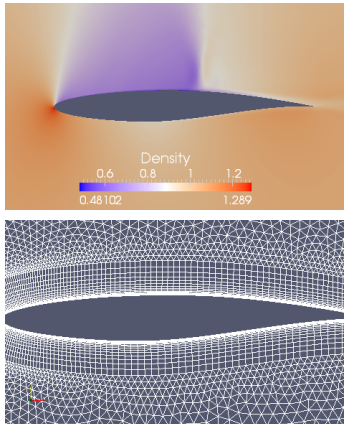


Figure 9: RAE-2822: Density profile and mesh.

- Transonic NACA-0012
($M_\infty = 0,8$; $Re = 6,5 \times 10^6$; $\alpha = 1,25^\circ$)

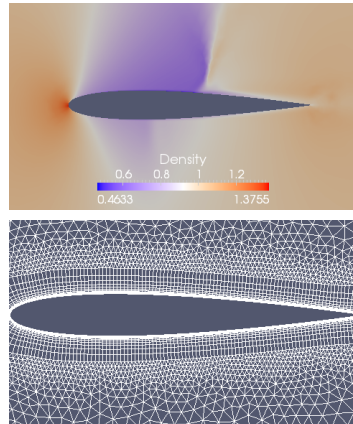
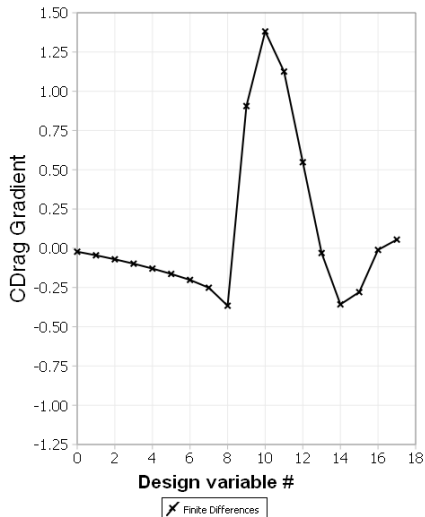
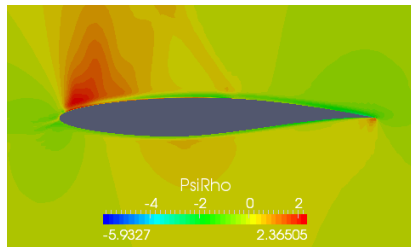
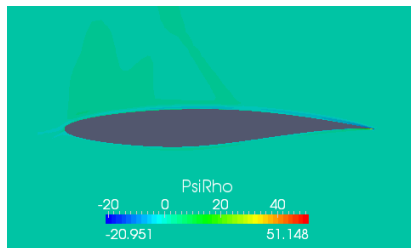
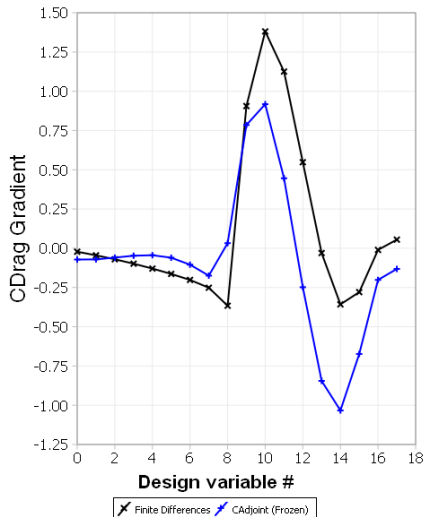
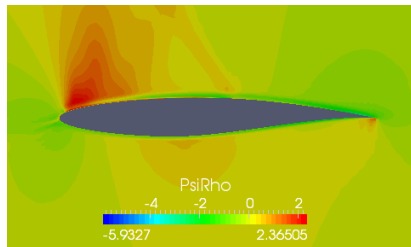
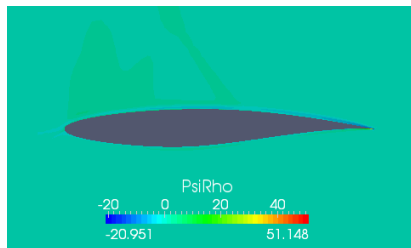


Figure 10: NACA-0012: Density profile and mesh.

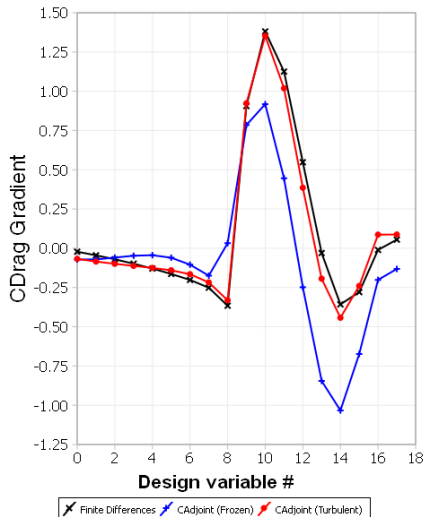
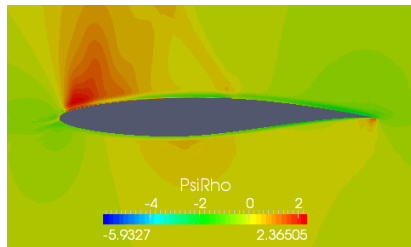
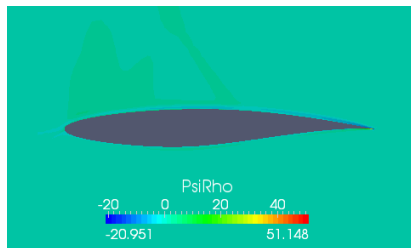
Numerical test 1: Transonic RAE-2822



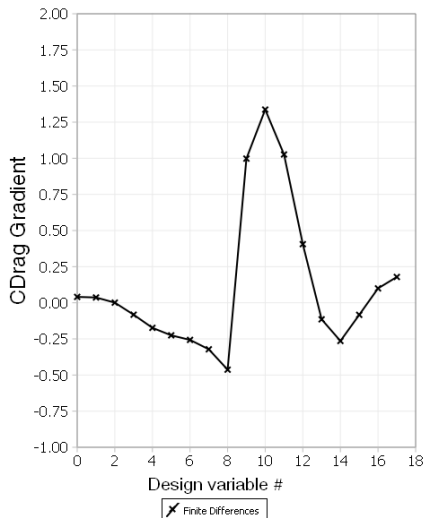
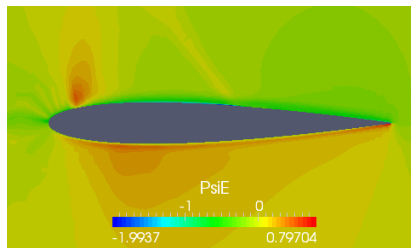
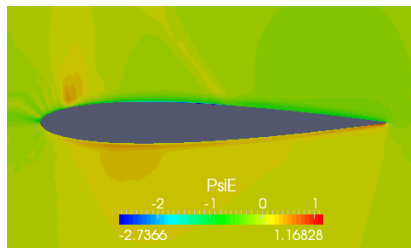
Numerical test 1: Transonic RAE-2822



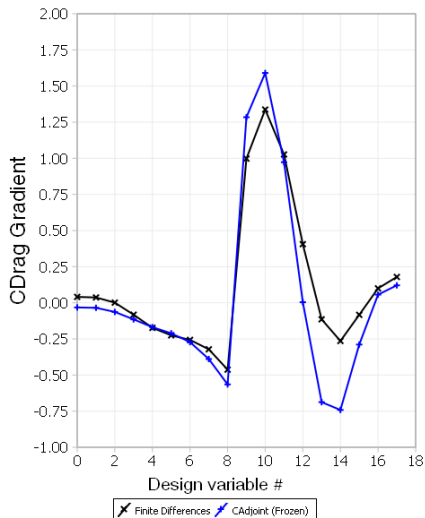
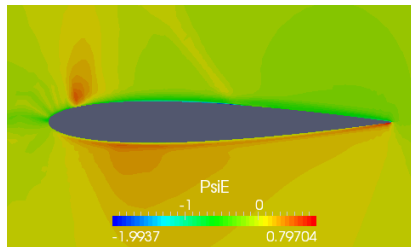
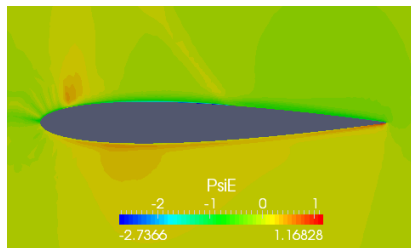
Numerical test 1: Transonic RAE-2822



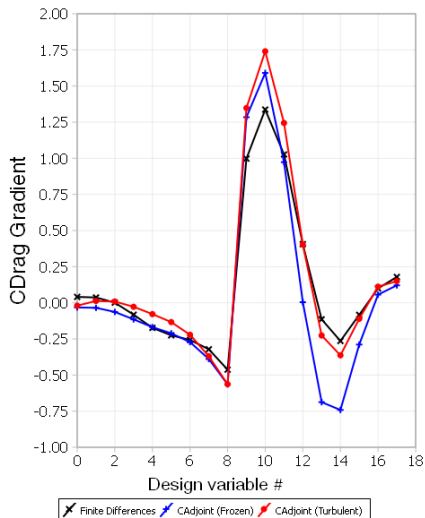
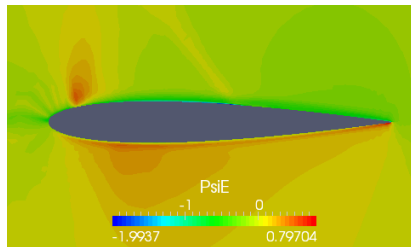
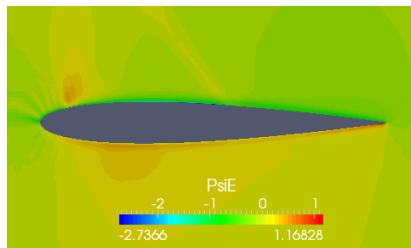
Numerical test 2: Transonic NACA-0012



Numerical test 2: Transonic NACA-0012



Numerical test 2: Transonic NACA-0012



Numerical test 3: 2D unconstrained drag minimization using adjoint RANS

The goal of this academic problem is to reduce the drag of a RAE-2822 profile, by means of modifications of its surface. A total of 38 Hicks–Henne bump functions have been used as design variables.

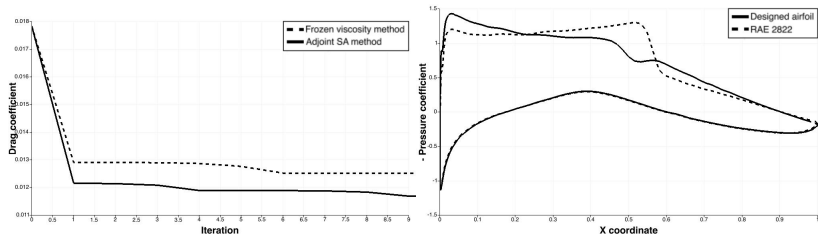


Figure 11: Optimization convergence history, adjoint method vs. frozen viscosity (left). Pressure coefficient distribution, original configuration and final design (right).

Outline

- 1 Introduction
 - Optimal design in aerodynamics
 - Alternatives for sensitivity calculations
- 2 Design Using the Euler Equations
- 3 Design Using the RANS Equations
 - Spalart-Allmaras Turbulence Model
- 4 Continuous adjoint for the Spalart–Allmaras model
 - Analytical formulation
 - Transonic RAE-2822
 - Transonic NACA-0012
 - Optimization of a transonic airfoil
- 5 Conclusions

Conclusions

- Continuous adjoint formulations for both the Euler and Reynolds-Averaged Navier-Stokes equations can be derived.
- Significant care required to obtain highly-accurate gradients (cannot freeze the eddy viscosity in RANS models).
- Automating the derivation and enabling the use of arbitrary cost functions is desirable (see next lecture).
- Powerful tool for shape optimization.