VOLKSWAGEN

AKTIENGESELLSCHAFT

KONZERNFORSCHUNG

Adjoint theory & Solver in OpenFOAM

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MARIE CURIE ACTIONS

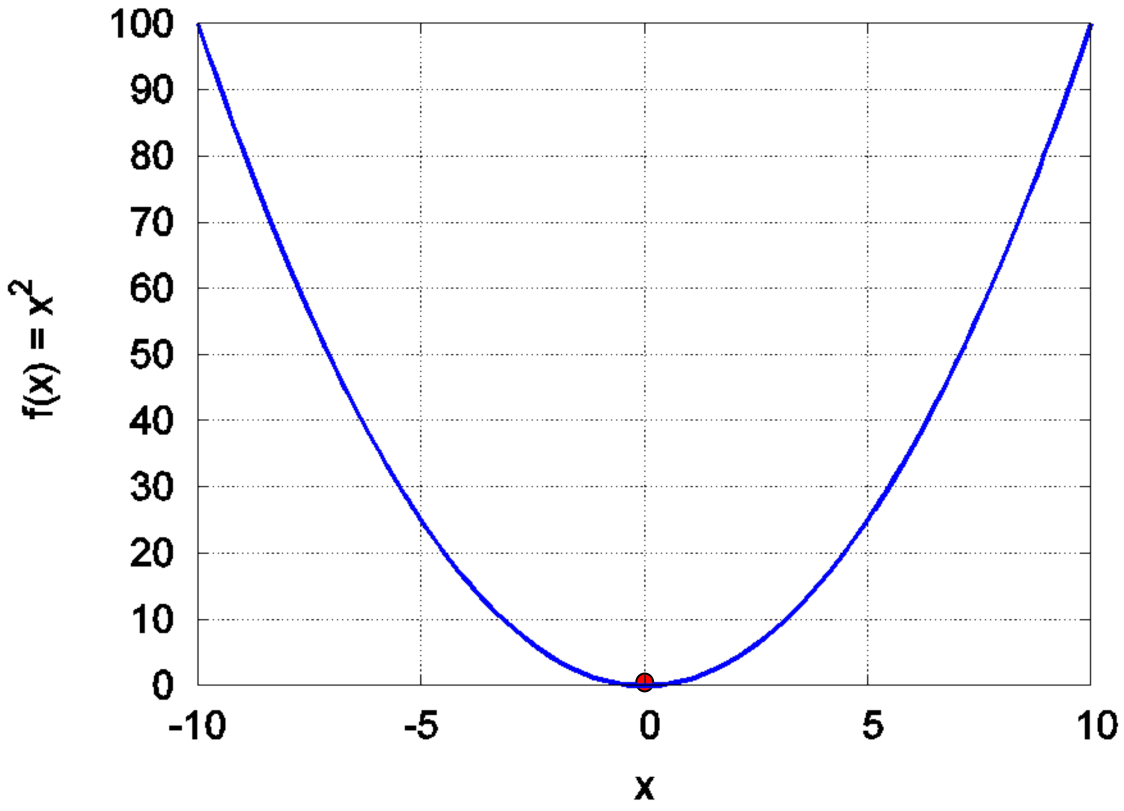
AGENDA

- Adjoint theory:
  - Numerical Optimisation
  - Why do we need the adjoints?
  - Continuous adjoint formulation

- OpenFOAM Adjoint Solver:
  - Our baseline: *adjointShapeOptimizationFoam (version 2.3.1)*
  - Enhance the code
  - Applications:
    - pitzDaily
    - Airfoil 2D

INTRODUCTION

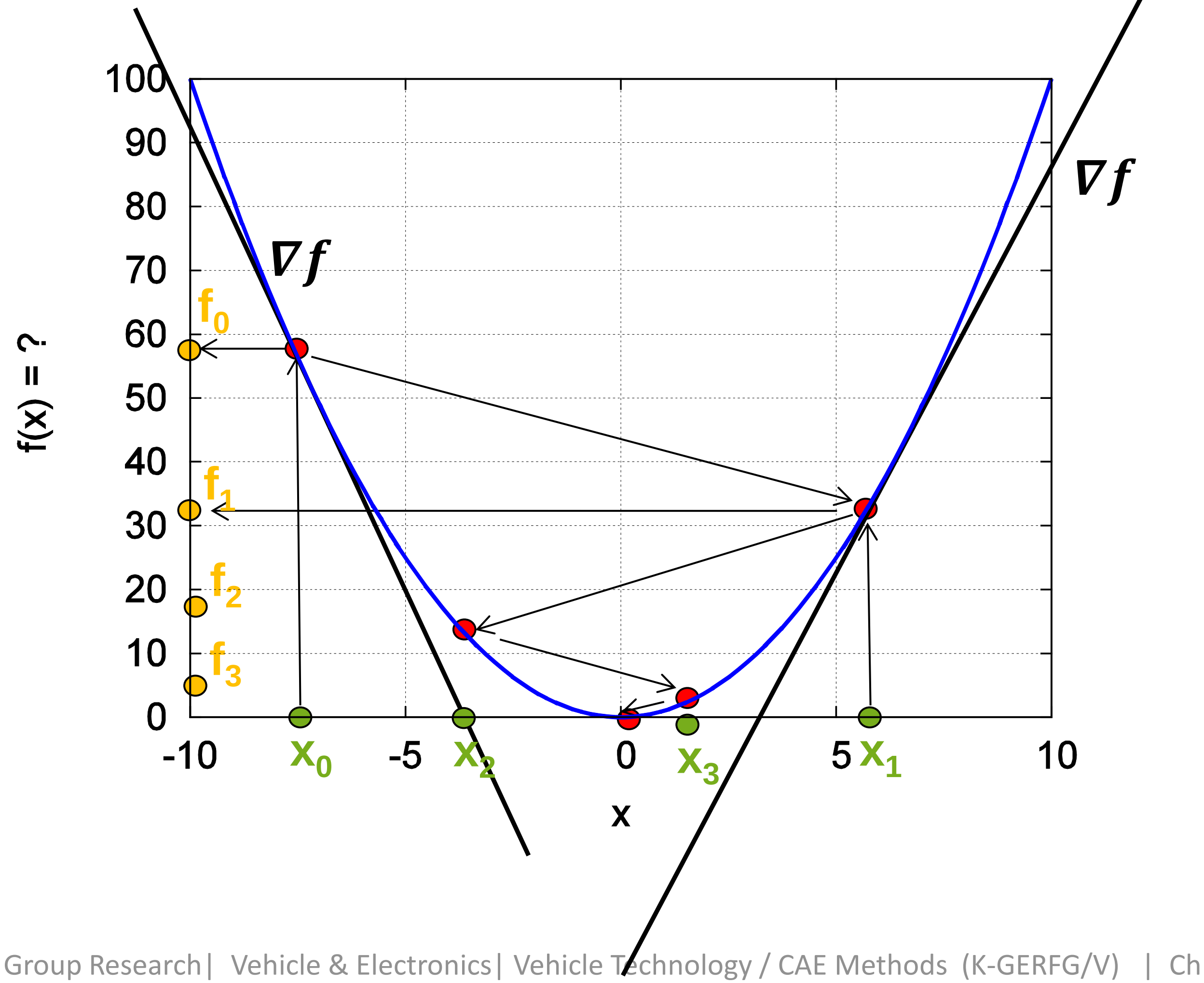
NUMERICAL OPTIMISATION



- Find the minimum of f(x)
- Analytical expression
- Here: $\nabla f = 2x$, $x_{min} = 0$

INTRODUCTION

NUMERICAL OPTIMISATION



- In the computational world the analytic functions are not known
- A simulation is a black box with specific **inputs** and **outputs** (i.e. Input: Car geometry, flow conditions – Output: Flow field, drag force)
- To optimise an output (**Objective Function**) with respect to an input (**Design Variables**) we need the **gradient**
- An **accurate** and **fast** way to compute the gradient is needed!!
- A way is with Finite Differences:

$$\frac{df}{dx} = \frac{f_+ - f_-}{x_+ - x_-}$$

ADJOINT METHOD

INTRODUCTION

- Primal Equations

$$\vec{R} = \vec{R}\left(\vec{V}, \vec{b}\right) = \vec{0}$$

- Objective Function

$$F = F\left(\vec{V}, \vec{b}\right)$$

- Differentiation of these:

$$\frac{\delta F}{\delta \vec{b}} = \frac{\partial F}{\partial \vec{b}} + \frac{\partial F}{\partial \vec{V}} \frac{\delta \vec{V}}{\delta \vec{b}}$$

$$\begin{aligned} \frac{\delta \vec{R}}{\delta \vec{b}} &= \frac{\partial \vec{R}}{\partial \vec{b}} + \frac{\partial \vec{R}}{\partial \vec{V}} \frac{\delta \vec{V}}{\delta \vec{b}} = 0 \\ &= \frac{\partial \vec{R}}{\partial \vec{b}} + A \frac{\delta \vec{V}}{\delta \vec{b}} = 0 \end{aligned}$$

ADJOINT METHOD

INTRODUCTION

- Direct Problem

$$\frac{\delta \vec{V}}{\delta \vec{b}} = A^{-1} \frac{\partial \vec{R}}{\partial \vec{b}}$$

$$\frac{\delta F}{\delta \vec{b}} = \frac{\partial F}{\partial \vec{b}} + \frac{\partial F}{\partial \vec{V}} \frac{\delta \vec{V}}{\delta \vec{b}}$$

- Adjoint Problem

$$\frac{\delta F}{\delta \vec{b}} = \frac{\partial F}{\partial \vec{b}} - \underline{\frac{\partial F}{\partial \vec{V}} A^{-1}} \frac{\partial \vec{R}}{\partial \vec{b}}$$

$$\vec{U}^T = -\frac{\partial F}{\partial \vec{V}} A^{-1}$$

$$\frac{\delta F}{\delta \vec{b}} = \frac{\partial F}{\partial \vec{b}} + \vec{U} \frac{\partial \vec{R}}{\partial \vec{b}}$$

CONTINUOUS ADJOINT FORMULATION

- Navier-Stokes Equations:

$$R^p = -\frac{\partial v_j}{\partial x_j} = 0$$

$$R_i^v = v_j \frac{\partial v_i}{\partial x_j} - \frac{\partial}{\partial x_j}\left[(\nu+\nu_t)\left(\frac{\partial v_i}{\partial x_j}+\frac{\partial v_j}{\partial x_i}\right)\right] + \frac{\partial p}{\partial x_i} = 0\ , \qquad i = 1, 2(, 3)$$

- Generic objective Function

$$F = \int_S F_{S_i} n_i dS + \int_\Omega F_\Omega d\Omega$$

- Augmented objective functions

$$F_{aug} = F + \int_\Omega u_i R_i^v d\Omega + \int_\Omega q R^p d\Omega$$

CONTINUOUS ADJOINT FORMULATION

- Differentiation of the augmented function:

$$\frac{\delta F_{aug}}{\delta b_n} = \frac{\delta F}{\delta b_n} + \frac{\delta}{\delta b_n}\int_\Omega u_i R_i^v d\Omega + \frac{\delta}{\delta b_n}\int_\Omega q R^p d\Omega$$

$$= \frac{\delta F}{\delta b_n} + \int_\Omega u_i \frac{\partial R_i^v}{\partial b_n} d\Omega + \int_\Omega q \frac{\partial R^p}{\partial b_n} d\Omega + \int_S (u_i R_i^v + q R^p) n_k \frac{\delta x_k}{\delta b_n} dS$$

- where:

$$\frac{\partial R^p}{\partial b_n} = -\frac{\partial}{\partial x_j}\left(\frac{\partial v_j}{\partial b_n}\right)$$

$$\frac{\partial R_i^v}{\partial b_n} = \frac{\partial v_j}{\partial b_n}\frac{\partial v_i}{\partial x_j} + v_j \frac{\partial}{\partial x_j}\left(\frac{\partial v_i}{\partial b_n}\right) - \frac{\partial}{\partial x_j}\left[(\nu + \nu_t)\frac{\partial}{\partial b_n}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)\right] + \frac{\partial}{\partial x_i}\left(\frac{\partial p}{\partial b_n}\right)$$

CONTINUOUS ADJOINT FORMULATION

- Product Rule:

$$\frac{\partial}{\partial x_i}(fF_i) = \frac{\partial f}{\partial x_i}F_i + f\frac{\partial F_i}{\partial x_i}$$

- Green-Gauss theorem:

$$\iiint_V \frac{\partial F_i}{\partial x_i} dV = \oiint_S F_i n_i dS$$

CONTINUOUS ADJOINT FORMULATION

- Applying these rules:

$$\int_{\Omega} -q\frac{\partial}{\partial x_j}\left(\frac{\partial v_j}{\partial b_n}\right) d\Omega = -\int_{S} q\frac{\partial v_j}{\partial b_n} n_j dS + \int_{\Omega} \frac{\partial q}{\partial x_j}\frac{\partial v_j}{\partial b_n} d\Omega$$

$$\frac{\partial}{\partial x_i}(fF_i) = \frac{\partial f}{\partial x_i}F_i + f\frac{\partial F_i}{\partial x_i}$$

$$\iiint_V \frac{\partial F_i}{\partial x_i} dV = \oiint_S F_i n_i dS$$

CONTINUOUS ADJOINT FORMULATION

- Applying these rules:

$$\int_\Omega u_i \frac{\partial v_i}{\partial x_j}\frac{\partial v_j}{\partial b_n} d\Omega + \int_\Omega u_i v_j \frac{\partial}{\partial x_j}\left(\frac{\partial v_i}{\partial b_n}\right) d\Omega =$$

$$\int_\Omega u_j \frac{\partial v_j}{\partial x_i}\frac{\partial v_i}{\partial b_n} d\Omega + \int_S u_i v_j n_j \frac{\partial v_i}{\partial b_n} dS - \int_\Omega \frac{\partial}{\partial x_j}(u_i v_j)\frac{\partial v_i}{\partial b_n} d\Omega$$

$$
\begin{aligned}
\frac{\delta F_{aug}}{\delta b_n} = & \int_S \left[u_i v_j n_j + (\nu + \nu_t)\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) n_j - q n_i + \frac{\partial F_{S_k}}{\partial v_i} n_k + \acute{F}^v_{S,i} \right] \frac{\partial v_i}{\partial b_n} dS \\
& + \int_S \left(u_j n_j + \frac{\partial F_{S_i}}{\partial p} n_i + \acute{F}^p_S \right) \frac{\partial p}{\partial b_n} dS + \int_S \left(-u_i n_j + \frac{\partial F_{S_k}}{\partial \tau_{ij}} n_k \right) \frac{\partial \tau_{ij}}{\partial b_n} dS \\
& + \int_{S_{W_p}} n_i \frac{\partial F_{S_i}}{\partial x_m} n_m \frac{\delta x_k}{\delta b_n} n_k dS + \int_{S_{W_p}} F_{S_i} \frac{\delta n_i}{\delta b_n} dS + \int_{S_{W_p}} F_{S_i} n_i \frac{\delta (dS)}{\delta b_n} \\
& + \int_{S_{W_p}} \left(u_i R^v_i + q R^p + F_\Omega \right) \frac{\delta x_k}{\delta b_n} n_k dS \\
& + \int_\Omega \left\{ u_j \frac{\partial v_j}{\partial x_i} - \frac{\partial (v_j u_i)}{\partial x_j} - \frac{\partial}{\partial x_j}\left[(\nu + \nu_t)\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] + \frac{\partial q}{\partial x_i} + \acute{F}^v_{\Omega,i} \right\} \frac{\partial v_i}{\partial b_n} d\Omega \\
& + \int_\Omega \left(-\frac{\partial u_j}{\partial x_j} + \acute{F}^p_\Omega \right) \frac{\partial p}{\partial b_n} d\Omega
\end{aligned}
$$

"*Adjoint Methods for Turbulent Flows, Applied to Shape or Topology Optimization and Robust Design*", E. Papoutsis-Kiachagias, PhD Thesis

CONTINUOUS ADJOINT FORMULATION

- Field Adjoint Equations

$$R^q = -\frac{\partial u_j}{\partial x_j} + \acute{F}_{\Omega}^{p} = 0$$

$$R_i^u = u_j \frac{\partial v_j}{\partial x_i} - \frac{\partial (v_j u_i)}{\partial x_j} - \frac{\partial}{\partial x_j}\left[(\nu + \nu_t)\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] + \frac{\partial q}{\partial x_i} + \acute{F}_{\Omega,i}^{v} = 0 \;,\quad i = 1, 2(, 3)$$

CONTINUOUS ADJOINT FORMULATION

- Boundary conditions at inlet:

$$u_j n_j = u_{\langle n \rangle} = -\frac{\partial F_{S_{I,i}}}{\partial p} n_i - \acute{F}^{p}_{S_I}$$

$$u^{I}_{\langle t \rangle} = \frac{\partial F_{S_{I,k}}}{\partial \tau_{ij}} n_k t^{I}_i n_j + \frac{\partial F_{S_{I,k}}}{\partial \tau_{ij}} n_k t^{I}_j n_i$$

$$u^{II}_{\langle t \rangle} = \frac{\partial F_{S_{I,k}}}{\partial \tau_{ij}} n_k t^{II}_i n_j + \frac{\partial F_{S_{I,k}}}{\partial \tau_{ij}} n_k t^{II}_j n_i$$

CONTINUOUS ADJOINT FORMULATION

- Boundary condition at outlet:

$$q = u_{\langle n \rangle} v_{\langle n \rangle} + 2(\nu + \nu_t)\frac{\partial u_{\langle n \rangle}}{\partial n} + \frac{\partial F_{S_{O,k}}}{\partial v_i} n_k n_i + \acute{F}^v_{S_{O,i}} n_i = 0$$

$$v_n u^l_{\langle t \rangle} + (\nu + \nu_t)\left(\frac{\partial u^l_{\langle t \rangle}}{\partial n} + \frac{\partial u_{\langle n \rangle}}{\partial t^l}\right) + \frac{\partial F_{S_{O,k}}}{\partial v_i} n_k t^l_i + \acute{F}^v_{S_{O,i}} t^l_i = 0$$

CONTINUOUS ADJOINT FORMULATION

- Boundary condition at walls:

$$u_{\langle n\rangle} = -\frac{\partial F_{S_{W,i}}}{\partial p} n_i - \acute{F}^{p}_{S_W}$$

$$u^{I}_{\langle t\rangle} = \frac{\partial F_{S_{W,k}}}{\partial \tau_{ij}} n_k t^{I}_{i} n_j + \frac{\partial F_{S_{W,k}}}{\partial \tau_{ij}} n_k t^{I}_{j} n_i$$

$$u^{II}_{\langle t\rangle} = \frac{\partial F_{S_{W,k}}}{\partial \tau_{ij}} n_k t^{II}_{i} n_j + \frac{\partial F_{S_{W,k}}}{\partial \tau_{ij}} n_k t^{II}_{j} n_i$$

- Sensitivity derivatives:

$$\frac{\delta F_{aug}}{\delta b_n} = -\int_{S_{W_p}} \left[(\nu+\nu_t)\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)n_j - q n_i + \frac{\partial F_{S_{W_p,k}}}{\partial v_i}n_k + \acute{F}^{v}_{S_{W_p,i}}\right]\frac{\partial v_i}{\partial x_k}n_k\frac{\delta x_m}{\delta b_n}n_m dS$$
$$+\int_{S_{W_p}} n_i \frac{\partial F_{S_{W_p,i}}}{\partial x_m}n_m\frac{\delta x_k}{\delta b_n}n_k dS + \int_{S_{W_p}} F_{S_{W_p,i}}\frac{\delta n_i}{\delta b_n}dS + \int_{S_{W_p}} F_{S_{W_p,i}}n_i\frac{\delta (dS)}{\delta b_n}$$
$$+\int_{S_{W_p}} (u_i R^v_i + q R^p + F_\Omega)\frac{\delta x_k}{\delta b_n}n_k dS$$
$$-\int_{S_{W_p}} \left[\left(-u_{\langle n\rangle} + \frac{\partial F_{S_{W_p,k}}}{\partial \tau_{lm}}n_k n_l n_m\right)\left(\tau_{ij}\frac{\delta (n_i n_j)}{\delta b_n} + \frac{\partial \tau_{ij}}{\partial x_m}n_m\frac{\delta x_k}{\delta b_n}n_k n_i n_j\right)\right] dS$$
$$-\int_{S_{W_p}} \left[\frac{\partial F_{S_{W_p,k}}}{\partial \tau_{lm}}n_k t^I_l t^I_m\left(\tau_{ij}\frac{\delta (t^I_i t^I_j)}{\delta b_n} + \frac{\partial \tau_{ij}}{\partial x_m}n_m\frac{\delta x_k}{\delta b_n}n_k t^I_i t^I_j\right)\right] dS$$
$$-\int_{S_{W_p}} \left[\left(\frac{\partial F_{S_{W_p,k}}}{\partial \tau_{lm}}n_k (t^{II}_l t^I_m + t^I_l t^{II}_m)\right)\left(\tau_{ij}\frac{\delta (t^{II}_i t^I_j)}{\delta b_n} + \frac{\partial \tau_{ij}}{\partial x_m}n_m\frac{\delta x_k}{\delta b_n}n_k t^{II}_i t^I_j\right)\right] dS$$
$$-\int_{S_{W_p}} \left[\frac{\partial F_{S_{W_p,k}}}{\partial \tau_{lm}}n_k t^{II}_l t^{II}_m\left(\tau_{ij}\frac{\delta (t^{II}_i t^{II}_j)}{\delta b_n} + \frac{\partial \tau_{ij}}{\partial x_m}n_m\frac{\delta x_k}{\delta b_n}n_k t^{II}_i t^{II}_j\right)\right] dS$$

CONTINUOUS ADJOINT FORMULATION

TOPOLOGY OPTIMISATION

- Navier-Stokes for topology optimisation:

$$R^p = -\frac{\partial v_j}{\partial x_j} = 0$$

$$R_i^v = v_j \frac{\partial v_i}{\partial x_j} - \frac{\partial}{\partial x_j}\left[(\nu+\nu_t)\left(\frac{\partial v_i}{\partial x_j}+\frac{\partial v_j}{\partial x_i}\right)\right] + \frac{\partial p}{\partial x_i} + \underbrace{\alpha v_i}_{T_{a,v}} = 0$$

- Extra “porosity” term: $T_{a,v}$

CONTINUOUS ADJOINT FORMULATION

TOPOLOGY OPTIMISATION

- Field adjoint equations with porosity:

$$R^q = -\frac{\partial u_j}{\partial x_j} + \acute{F}^p_\Omega = 0$$

$$R^u_i = u_j \frac{\partial v_j}{\partial x_i} - \frac{\partial (v_j u_i)}{\partial x_j} - \frac{\partial}{\partial x_j}\left[(\nu + \nu_t)\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] + \frac{\partial q}{\partial x_i} + \acute{F}^v_{\Omega,i} + \underbrace{\alpha u_i}_{T_{a,u}} = 0$$

- Sensitivities wrt. porosity:

$$\frac{\delta F}{\delta \alpha} = \int_\Omega u_i v_i d\Omega$$

APPLICATIONS

PITZ DAILY

- Objective Function: Power Losses

$$F = \int_o \left[v_i n_i \left(\frac{1}{2} v^2 + p \right) \right] dS - \int_i \left[v_i n_i \left(\frac{1}{2} v^2 + p \right) \right] dS$$

- Field Adjoint Equations

$$\begin{aligned} R^q &= \frac{\partial u_i}{\partial x_i} = 0 \\ R_i^u &= u_j \frac{\partial v_j}{\partial x_i} - \frac{\partial (v_j u_i)}{\partial x_j} - \frac{\partial}{\partial x_j} \left[(\nu + \nu_t) \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] + \frac{\partial q}{\partial x_i} + \alpha u_i = 0 \end{aligned}$$

APPLICATIONS

PITZ DAILY

- Inlet boundary condition:

$$u_i = -v_j n_j n_i$$

- Outlet boundary condition:

$$q = u_j v_j + u_n v_n + (\nu + \nu_t)\frac{\partial u_n}{\partial x_j} n_j - \frac{1}{2} v^2 - u_n^2 - p$$

$$0 = u_t v_n + u_n v_n + (\nu + \nu_t)\frac{\partial u_t}{\partial x_j} n_j - v_n v_t$$

- Sensitivity derivatives:

$$\frac{\delta F}{\delta \alpha} = \int_\Omega u_i v_i d\Omega$$

APPLICATIONS

2D AIRFOIL

- Objective Function: Drag

$$F = \int_{S_w} \left[-(\nu + \nu_t) \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) + p\delta_j^i \right] n_j r_i dS$$

- Field Adjoint Equations

$$\begin{aligned} R^q &= \frac{\partial u_i}{\partial x_i} = 0 \\ R_i^u &= u_j \frac{\partial v_j}{\partial x_i} - \frac{\partial (v_j u_i)}{\partial x_j} - \frac{\partial}{\partial x_j} \left[(\nu + \nu_t) \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] + \frac{\partial q}{\partial x_i} = 0 \end{aligned}$$

APPLICATIONS

2D AIRFOIL

- Wall boundary condition:

$$u_i = -r_i$$

- Outlet boundary condition:

$$q = u_j v_j + u_n v_n + (\nu + \nu_t)\frac{\partial u_n}{\partial x_j} n_j$$

$$0 = u_t v_n + u_n v_n + (\nu + \nu_t)\frac{\partial u_t}{\partial x_j} n_j$$

- Sensitivity derivatives:

$$\frac{\delta F}{\delta x_n} = \int_{S_w} -(\nu + \nu_t)\frac{\partial u_i}{\partial x_j} n_j \frac{\partial v_i}{\partial x_k} n_k dS$$