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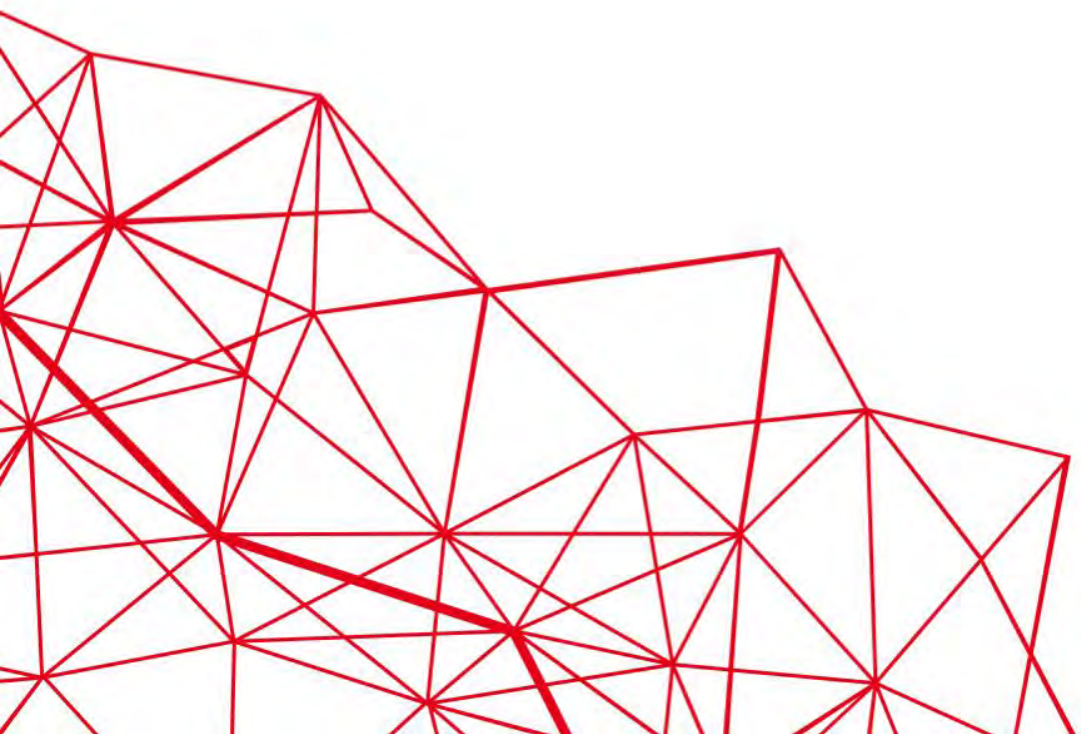

Data-Driven Techniques to Enhance and Supplement Computational Fluid Dynamics Prediction Capabilities

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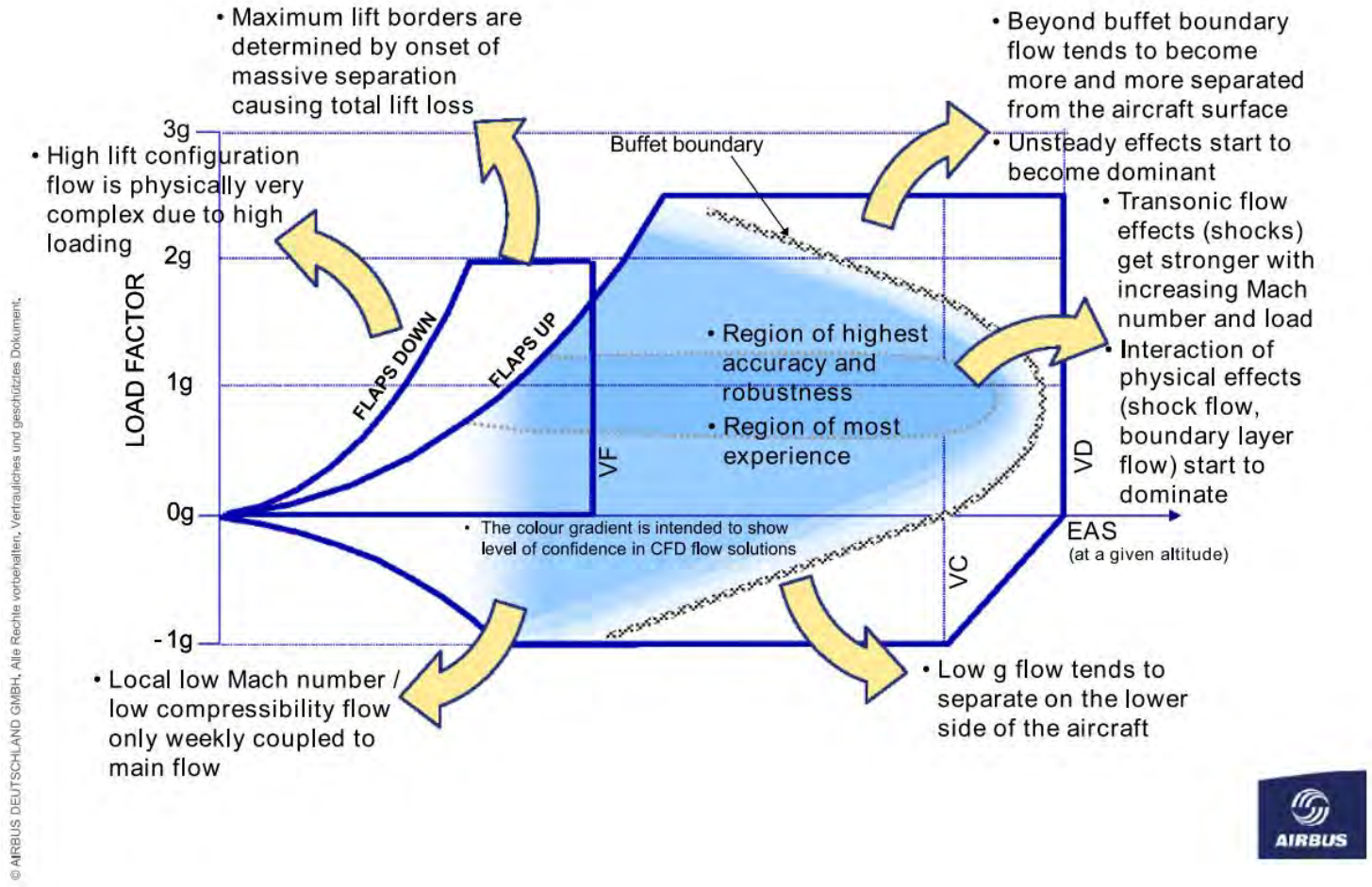
Outline

- Motivation
- SMARTy
- Methods to Supplement Computational Fluid Dynamics
- Methods to Enhance Computational Fluid Dynamics
- Conclusions & Future Work

Motivation

- CFD simulations – in particular RANS simulations – play an important role in modern aircraft design
- High-quality aerodynamic data hopefully enables better design
- Region of high accuracy and robustness is centered around the cruise point
- Computational cost is still a bottleneck for multi-query scenarios (e.g. optimization or loads analysis)



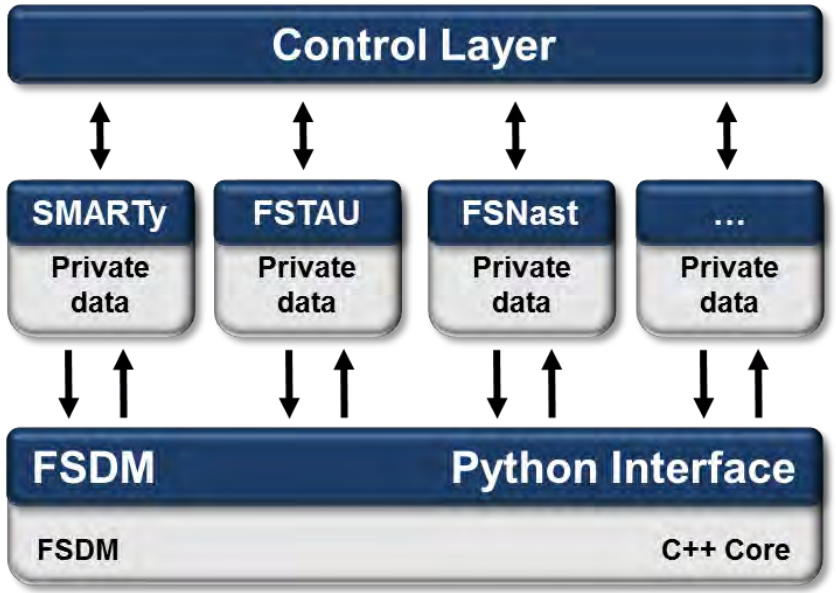
Estimation of CFD capabilities across the flight envelope [1]

[1] Abbas-Bayoumi, A., Becker, K. **An industrial view on numerical simulation for aircraft aerodynamic design**. J.Math.Industry 1, 10 (2011). https://doi.org/10.1186/2190-5983-1-10

Surrogate Modeling for AeRo Data Toolbox (SMARTy)

Key features

- Design of experiments
- Adaptive sampling
- Surrogate Modeling
- Hyperparameter optimization
- Variable-Fidelity Modeling
- Dimensionality reduction
- Reduced Order Modeling
- FlowSimulator “plug-in”, using FSDM & FSTAU functionalities
- Parallelized, partly differentiated, MKL, interfaces to Scikit-learn
- standalone version with use-case specific C-interface*



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Applications

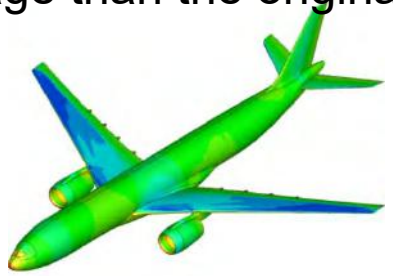
- Surrogate-based shape optimization
- Uncertainty quantification
- Robust & inverse design

- Fusing experimental + CFD data
- Optimal sensor placement
- Wind-tunnel corrections and support

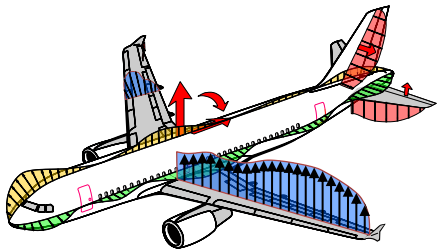
- Accelerating CFD computations
- Virtual flight testing
- Rapid aero-data & loads prediction across the flight envelope (and structural sizing in MDO context)

Motivation to Supplement Computational Fluid Dynamics

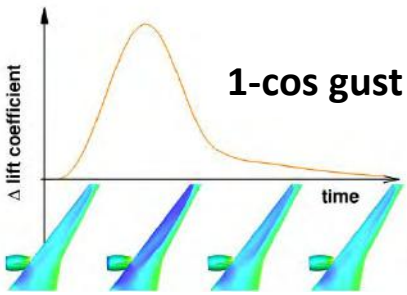
- From aircraft design to certification many **aerodynamic data** are needed for the entire flight envelope → pressure & shear stress distributions, global coefficients, derivatives from steady and unsteady simulations
- **Goal:** provide predictions of the aerodynamics based on **high-fidelity CFD** but with lower evaluation time and storage than the original CFD model → **ROMs**



LOADS



PERFORMANCES



HANDLING QUALITIES

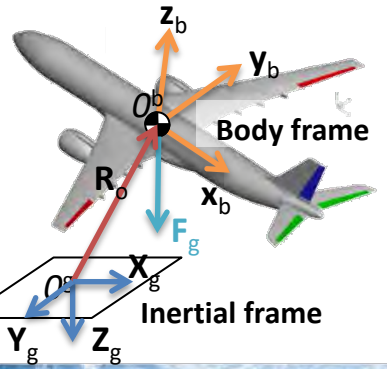
50 flight conditions (A)

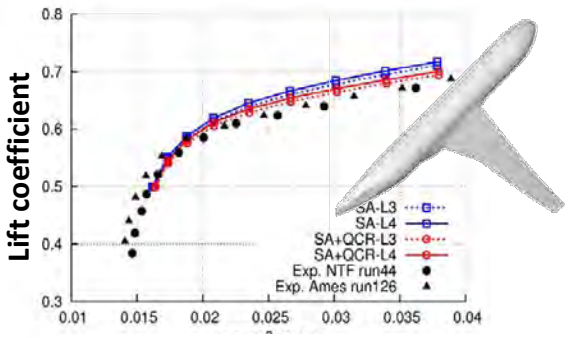
C: 4 control laws

M: 100 mass configs.

S: 5 maneuvers + 25 gust lengths

$\mathcal{O}(10^6)$ simulations





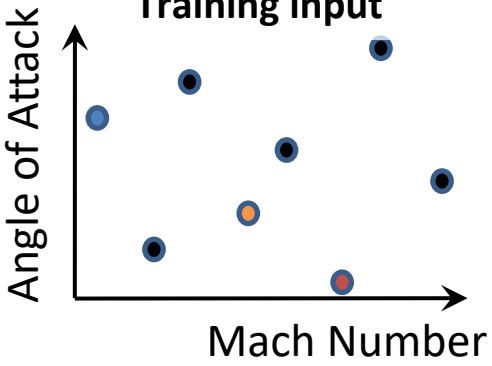
Idealized drag coefficient

DLR

Methodology

1

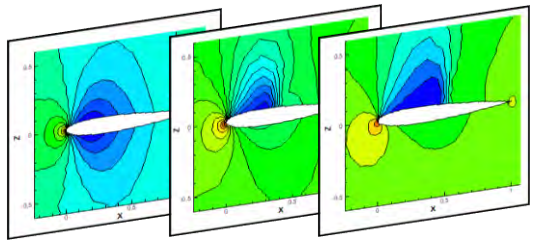
Training input



Define training points

2

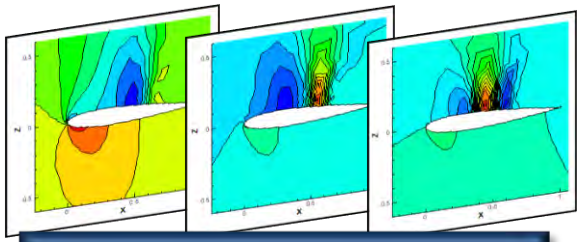
Training output



Compute training outputs with CFD

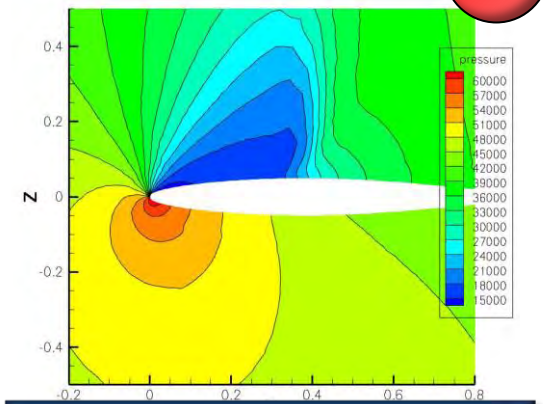
3

a) POD + Interpolation
b) Isomap + Residul Min
c) Neural Networks



Build a data-driven Model

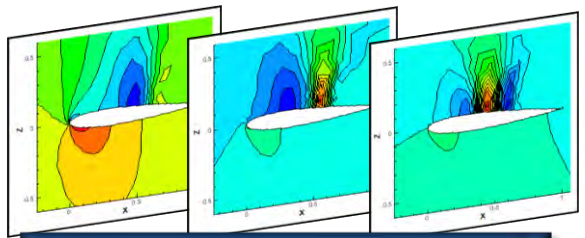
4



Flow prediction at untried condition

Methodology

a) POD + Interpolation
b) Isomap + Residual Min.
c) Neural Networks



Build data-driven Model

a) POD + Interpolation

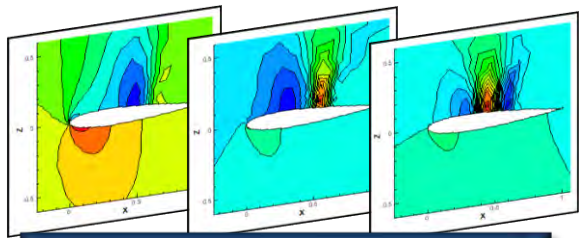
- Proper Orthogonal Decomposition for dimensionality reduction
- Gaussian Processes to interpolate on the latent space
- Non-intrusive, data-driven approach

\+ Works on surface data only
\+ Fast training and predictions
\+ Easy to implement and parallelize
\- Does not take any physical information into account
\- POD is inherently linear but CFD problems are typically not

POD + Interpolation can be seen as the standard baseline approach which is widely used in academia and industry

Methodology

a) POD + Interpolation
b) Isomap + Residual Min.
c) Neural Networks



Build data-driven Model

3

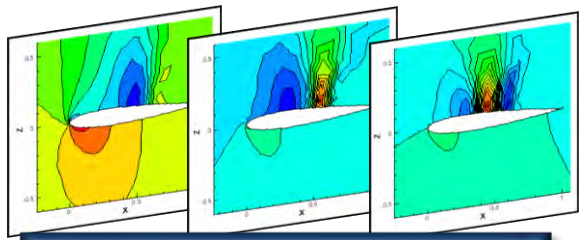
b) Isomap + Residual Minimization

- Isomap as Manifold Learning Technique is used for dim. reduction
  - Finds the closest solutions by searching on the manifold
- Solution are determined by minimizing the full or parts of the discretized residual
- Intrusive, physics-informed approach

\+ Takes physical knowledge into account
\+ Explores the solution space by searching the manifold for closest points
\+ Faster predictions compared to full CFD runs
\- Needs the full flow-state (at least in its current implementation)
\- Needs access to the underlying discretized residual

Methodology

a) POD + Interpolation
b) Isomap + Residual Min.
c) Neural Networks



Build data-driven Model

3

c) Neural Networks

- Building a neural network based on flow-state and surface location
  - Predicting one pressure coefficient for one point at the time
  - Greatly boosts the number of training points compared to predicting the full surface at once
- Non-intrusive, data-driven approach

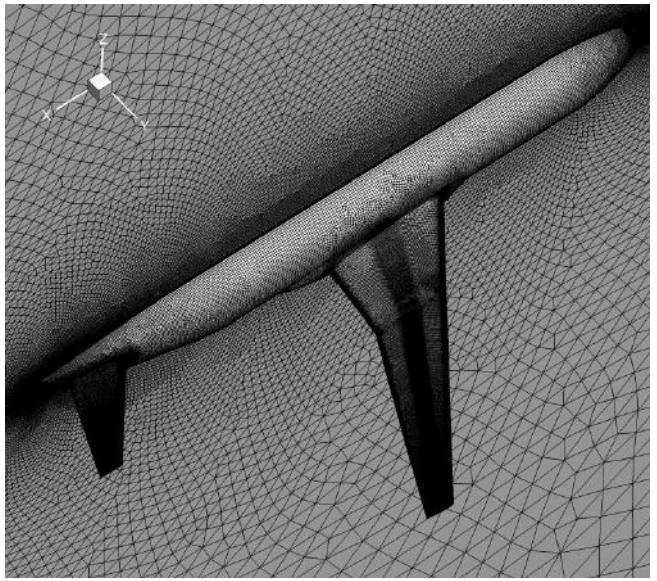
\+ Works on surface data only
\+ Capable of predicting also complex behavior
\- Large amount of architectures and parameters to be determined
\- High computational costs for training needed

In particular a fully connect MLP network is applied herein

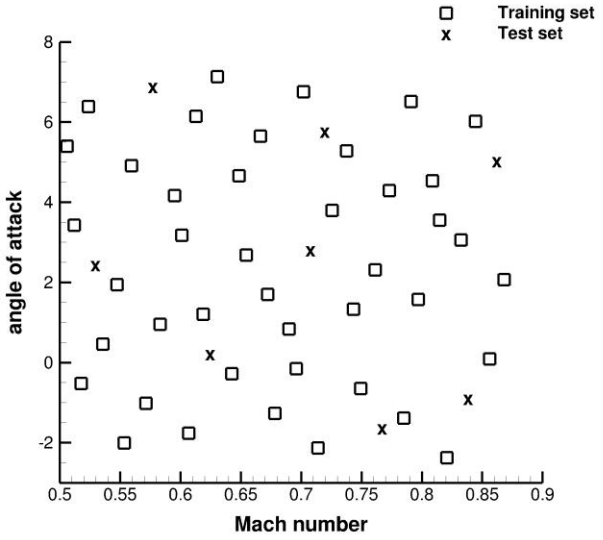
- 3 hidden layers with 500 neurons each
- ReLU as activation function
- Adam optimizer with roughly 600 epochs

Test Case NASA CRM

- The NASA CRM is a generic aircraft model for research
- Scaled to full scale and elastically deformed to obtain flight shape
- DLR-TAU Code solving the RANS equations with SA turbulence model
- Roughly 7 million grid nodes with 225 000 on the surface
- Varying angle of attack and Mach number
  - 42 snapshots as training dataset
  - 8 snapshots as test dataset

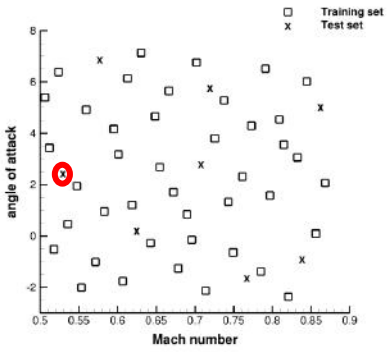


Computational grid around the aircraft

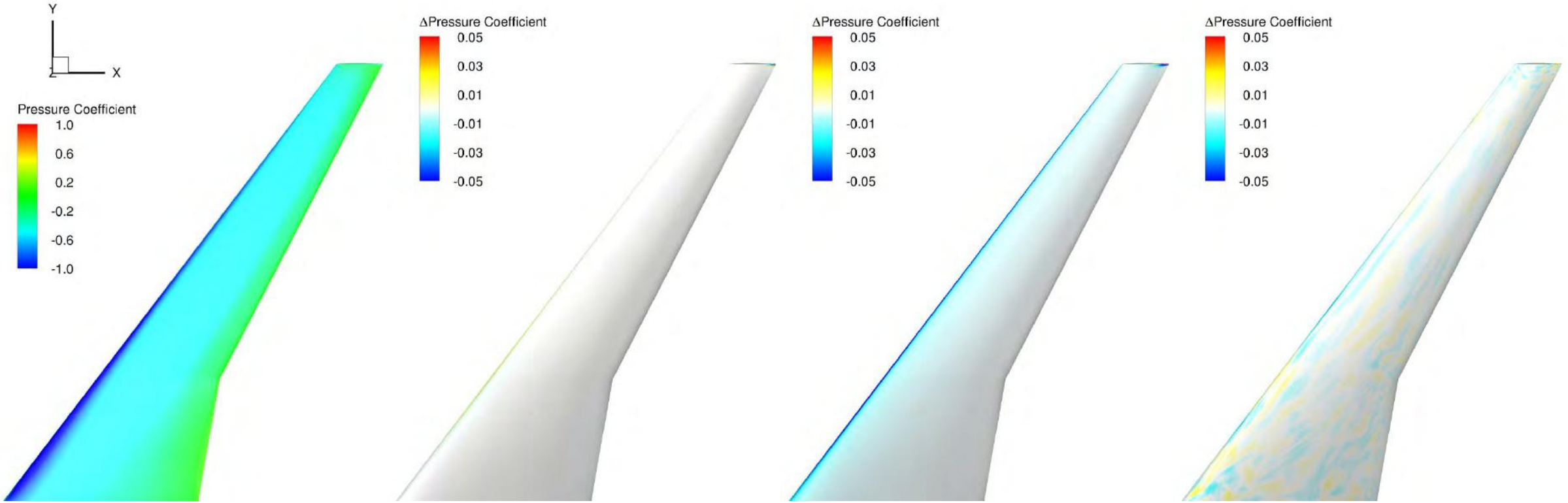


Training and Test data set

Results

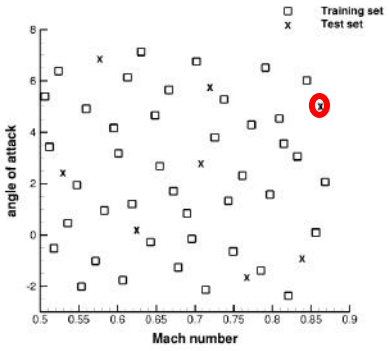


- Prediction at Mach = 0.52969 and AoA = 2.43827

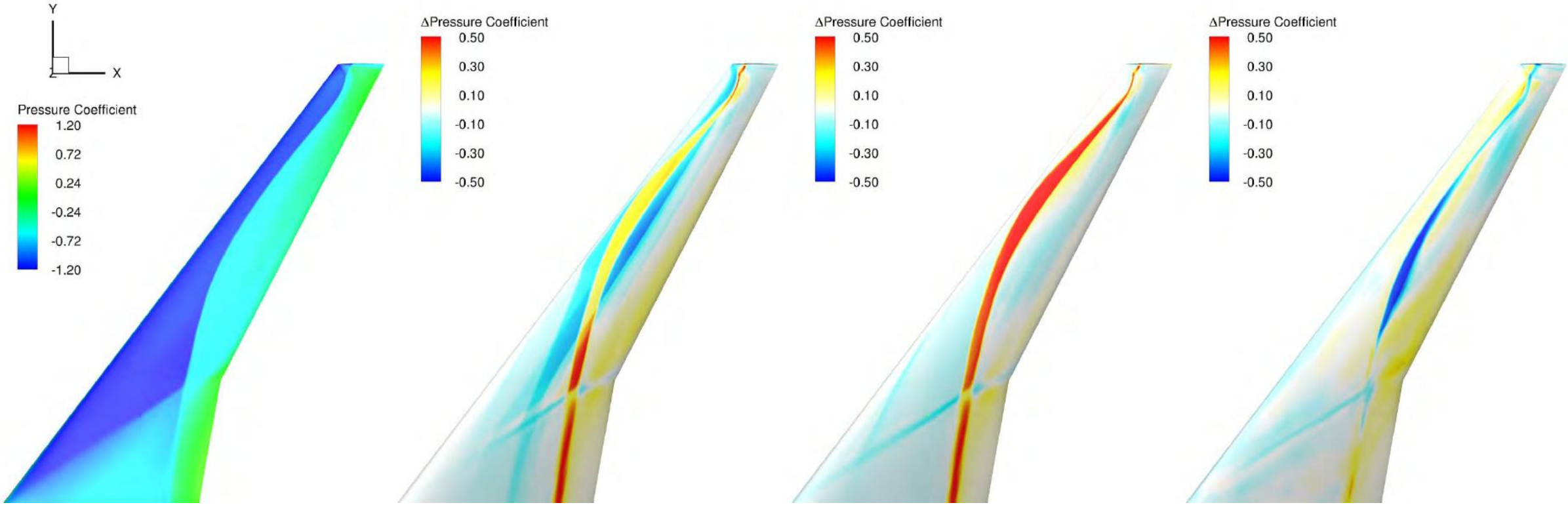


RANS Reference Solution | POD + I Solution | Isomap + Res. Min. Prediction | NN Prediction

Results



- Prediction at Mach = 0.86219 and AoA = 5.03086



RANS Reference Solution | POD + I Solution | Isomap + Res. Min. Prediction | NN Prediction

Motivation to Enhance Computational Fluid Dynamics

- DNS, LES are computationally expensive since all turbulent scales need to be resolved, experiments are expensive as well
- RANS are computationally cheaper since influence of turbulence on the mean flow is modeled and not all scales need to be resolved
- Turbulence models are often less precise, especially at the borders of the flight envelope

Methodology

How can high-fidelity data gathered from DNS, LES and experiments together with Machine Learning be used to improve existing Turbulence Models?

Idea:

- Augment the existing turbulence model (here: Spalart-Allmaras) by introducing a correction factor β:

$$\frac{D\tilde{\nu}}{Dt} = \beta P(\tilde{\nu}, U) - D(\tilde{\nu}) + T(\tilde{\nu}, U)$$

- For multiple cases, compute the optimal distributions for β so that the results from the RANS model match the high-fidelity reference data (Field Inversion)
- Using these β-distributions, find a function for β using Machine Learning
- Insert the ML-model in the augmented turbulence model and apply it to new cases

- Proposed by K. Duraisamy and colleagues, around 2015

Methodology

- The goal of Field Inversion is to modify β so that the results d_β from the RANS calculations with the augmented turbulence model match the results d_{ref} from the high-fidelity methods
- Thus, minimize the cost function

$$\mathcal{I}(\beta) = \frac{1}{2}\left(\sum_j^{N_{\text{ref}}}(d_{\text{ref},j} - d_{\beta,j})^2 + \lambda \sum_i^{N}(\beta_i - 1)^2\right)$$

- The second term of the cost function is a regularization since we have many DOFs (= number of cells)
- This is a constrained optimization problem, since the RANS-equations need to stay satisfied (R=0)
- For efficient optimization, a gradient-descent based method can be applied, since the gradient dI/dβ can be calculated efficiently using the adjoint method

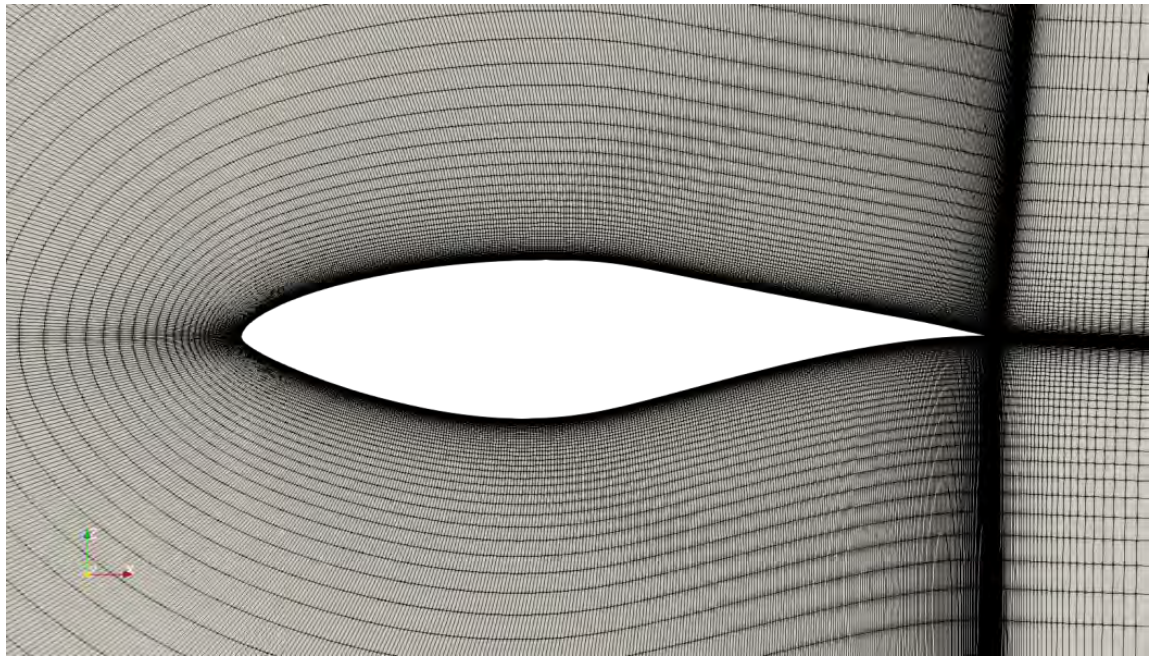
Methodology

- Field Inversion is only the first step to improve the turbulence model,
  - β-distributions is only valid for the respective cases

- A function $\beta(\eta_1, \eta_2, ...)$ depending on flow features $\eta_1, \eta_2, \ldots$ needs to be found
  - Use Machine Learning to determine such a function
  - Neural Networks are especially promising, since they can *approximate any limited function* (Universal Approximation Theorem)

Results: The S809 airfoil

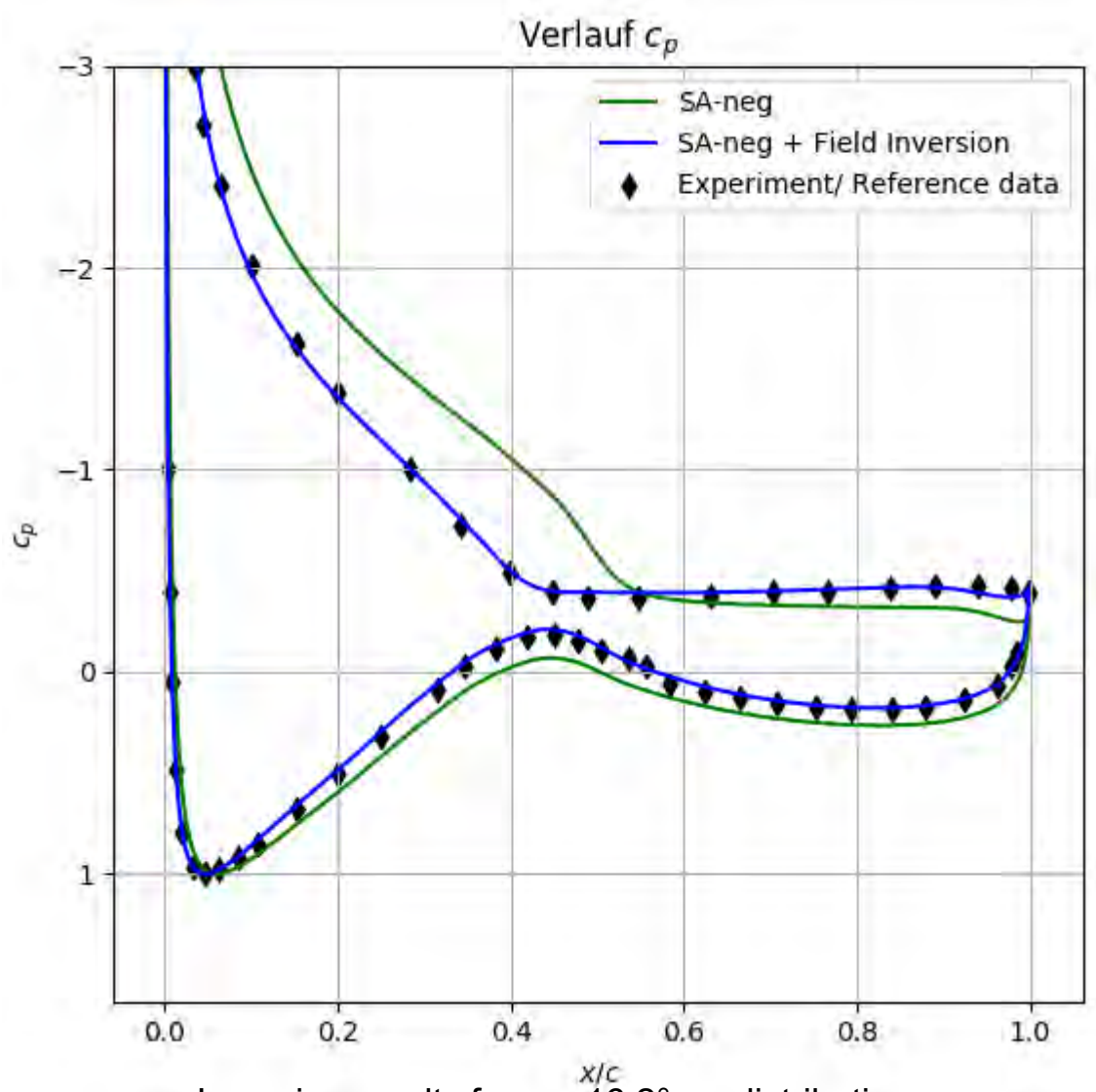
- The S809 is an airfoil for wind energy researched by NREL
- Reliable experimental data available for c_p and c_L at a wide range of angles of attack [3]
- Roughly 300 000 grid nodes
- Singh, Holland have used the S809 airfoil previously



Computational grid around the airfoil surface

Results: The S809 airfoil

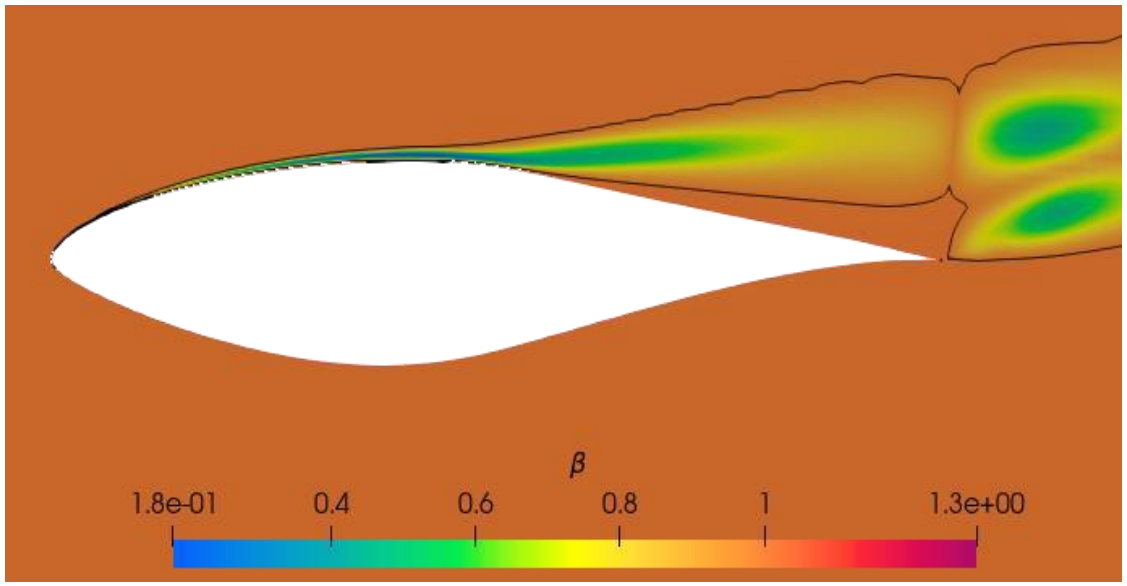
- Field Inversions were performed for α = 12.2°, 16.2° and 18.2°
- minimizing the difference of the c_p distributions between experiment and RANS simulation
- The experimental data can be matched almost perfectly
- Matching c_p also reduces the deviation in c_l e.g. from ~35% to ~4% for α = 16.2°



Inversion results for α = 16.2°, c_p-distribution

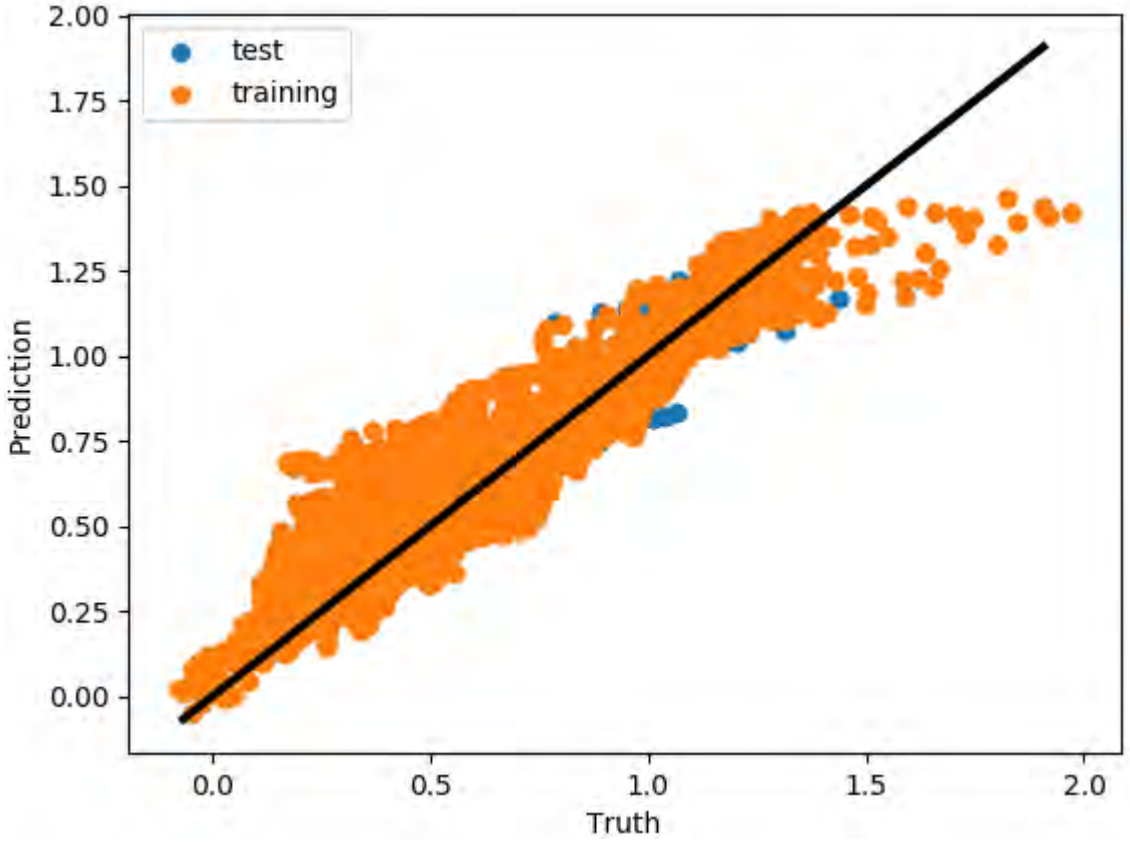
Results: The S809 airfoil

- Using the three datasets from the Inversion (α = 12.2°, 16.2°, 18.2°) but neglecting point with β = 1
- Training a Neural Network
- Neural Network
  - Fully connected, 2 layers à 200 neurons
  - ReLU and dropout
  - Adam – 200 epochs
  - Input features [2]: $\{\frac{P}{D}, \chi, \frac{|S|}{|\Omega|}, \frac{\mu_t|S_{ij}|}{1.5\tau_w}\}$
  - Target: β

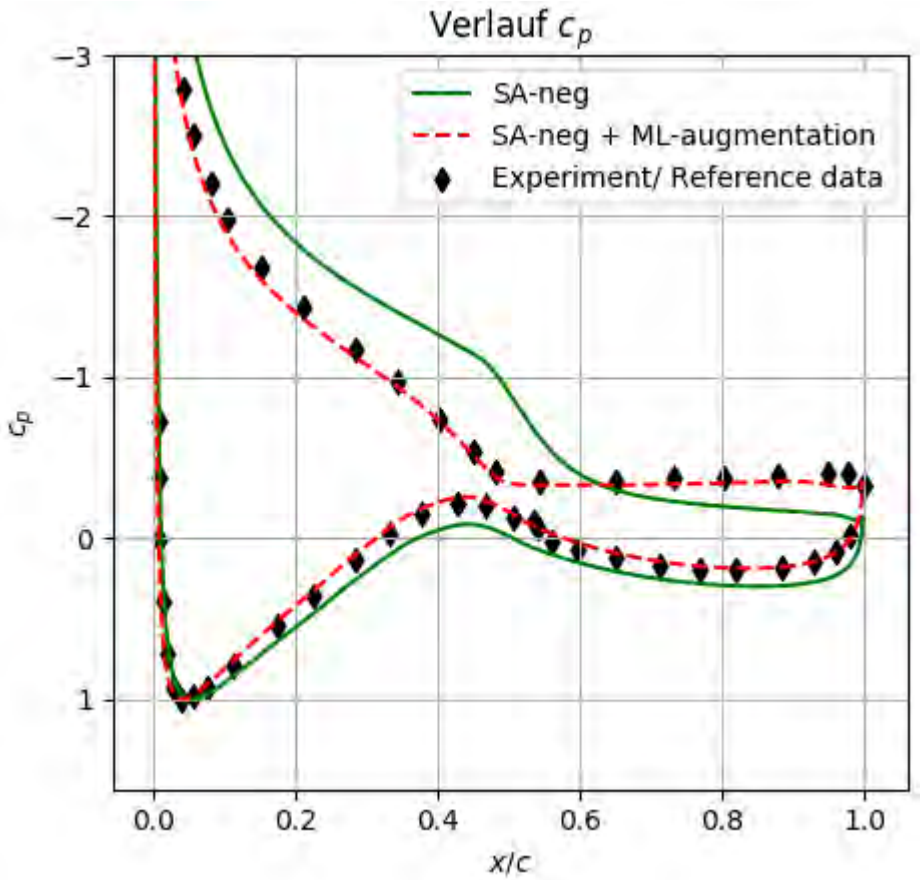


Inversion results for α = 16.2°, β-field

Results: The S809 airfoil



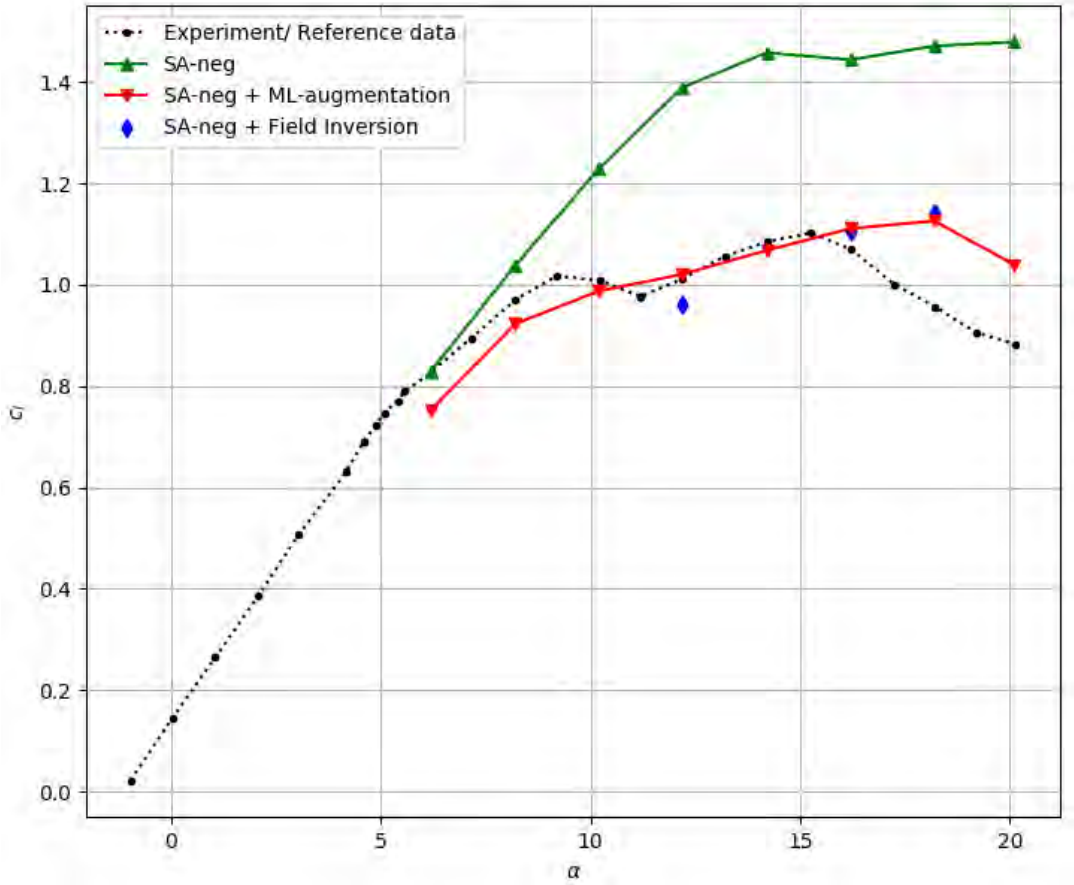
Ground truth vs Prediction, ML-model



RANS calculation with the ML-augmented Turbulence model, α = 14.2°

Results: The S809 airfoil

- The ML-augmented turbulence model greatly improves the RANS results in areas where c_l vs α is non-linear, i.e. where flow separation is dominant
- This is not only true for the datasets the ML-model was trained on (α = 12.2°, 16.2°, 18.2°), but also over a wider range (6.2° < α < 20.1°)
- Differences between match in c_p and c_l as a result of experimental data



Lift Coefficient over angle of attack for different modeling approaches

Conclusions

- Provided insight into DLRs work on data-driven techniques

1) Supplementing CFD capabilities by ML-based models for multi-query problems
    - Compared 3 different techniques
        a) POD + Interpolation
        b) Isomap + Residual Minimization
        c) Regression based on Neural Networks
    - Presented results for NASA CRM

2) Enhancing CFD capabilities by ML-based turbulence modeling
    - Revisited field inversion and ML step
    - Presented results for S809 airfoil

Future Work

- Next steps for the data-driven reduced order modeling part
  - Enabling residual minimization techniques on subset of points
  - Exploring different network architectures
  - Combining physical insights with neural networks

- Next steps for the data-driven turbulence modelling part
  - Investigations on the influence of the field inversion, i.e. the β-distribution due to
    - Regularization, type of cost function, amount of reference data available
  - Application of the FIML-approach to new test cases
  - Extensive data exploration and feature selection/ engineering