Data Augmented Design of Turbulence Modeling[1)]

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Abstract— As for the high Reynolds flow, aerodynamic design is mostly based on Reynolds Averaged Navier-Stocks equations (RANS). As introducing the ensemble average hypothesis, the accuracy of RANS equation is widely doubted in predicting the transition and flow separation, for example the laminar separation bubble or stalls under high angle of attack. This article takes an airfoil as an example and conducts a research on the data-augmented turbulence modeling design. Based on the high fidelity prior data from experiment, a spatially-varying term which will act as a multiplier of the viscous production term in Spalart-Allmaras model equation can be constructed using primal N-S flow and adjoint flow. In order to handle the issue of the extreme high dimension of this optimization problem (which is close to the number of grids), an adjoint method is used to solve the derivatives efficiently. The posterior result state that using a data-augmented turbulence modeling could predict the flow characteristics more accuracy, which can let the prediction of aerodynamic parameters like lift and drag more precise.

Keywords*—Data augmented, adjoint method, turbulence model*

1 INTRODUCTION

Computational fluid dynamics is widely used in physics and engineering problems such as aerodynamics and aerospace industry, weather simulation and environmental engineering. There are some of the computational methods such as Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES) which can provide relatively accurate solution. However, their calculation cost are expensive and require a long period of time consuming. From the consideration of affordability, Reynolds Averaged

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Navier-Stokes (RANS) equation is still the majority method in industrial and academic flow solvers. Through the introducing of ensembled average assumptions, explicit expression [2] and partial differential equation [3] are introduced to solve the Reynolds stress. The turbulent models, such as Spalart-Allmaras and Menter k-omega SST, model the spatio-temporal multiscale turbulent structures and significantly improve the efficiency of calculation.

Meanwhile, the ability of RANS model to perform a high-fidelity computation is restricted due to the introduction of the spatio-temporal assumption and the constrains of model parameters. The restriction can be state from two aspect, the first is that some of the fluid which included complex effects such as flow separation and large adverse pressure gradient can not be accurately modeled [4]. The second point is that the non-dimensional parameters are setting based on a small set of canonical problems and are of less generality when solving flows under different condition or geometrics. In addition, during the application, the selection of turbulence models requires personal judgement which relys on designers'engineering experiences.

As for the basic research of turbulent fluid, Prandtl-con-Karman's log theories [5] describe the local approximate solution on logarithmic region , but failed to provide a whole prediction of velocity and kinetic energy profile. Schaefer [6][7] conduct a sensitivity analysis on the S-A model closure coefficients. It was stated that the von Kaman constant (κ) and the turbulent Prandtl number (σ) play an important role on the changing of quantities uncertainty while the primary sources of uncertainty come from the formation of the model.

Early in the 20th century, Parneix[8] used DNS datasets to improve the terms in turbulence model such as the second moment closure. They modified the equation to improve the model accuracy. Most of the previous work for model discrepency improvement use data to calibrate the parameters in existing models such as S-A model. Recently, data augmented methods are used to address the model discrepancies. Xiao[9] computed the distribution of disturbance in the anisotropy Reynolds stress tensor based on DNS datasets. The disturbance to the anisotropic tensor is calculated with ensurance of realizability of the resulting perturbed stresses. The perturbations are reconstructed as a function of local flow variables.

Duraisamy[10] built a FIML approach that combined the flow inverse and machine learning. A specific objective function was used to quantificationally describe the model discrepency and a set of correction terms are embedded into the turbulence model to improve the model accuracy. The mapping relationship between flow field characteristics and correction terms is established by using neural network method, which can be used to improve the accuracy of turbulence model under different flow conditions.

Ling and Templeton [11] developed a machine learning classifier based on DNS and LES results to identify the turbulence in RANS models. They studied the flow field regions with significant deviations or irrational assumptions, and compared the training effects on certainty of different machine learning algorithms, such as support vector machine, decision tree and random forest. The results show that in the flow with different conditions, these classifiers can also identify the flow characteristics.

Wang [12] states that the large deviation of Reynolds stress is the main reason that limits the prediction accuracy of the RANS model. It is important to identify these differences for improving the RANS model. Based on the averaged flow field characteristics of DNS data, a random forest is established to reconstruct the Reynolds stress tensor. The reconstruction is based on the fully developed turbulence in square pipe and the flow field with large flow separation. After learning, the RANS calculation can obtain more accurate results than the base turbulence model in the flow field with different geometric conditions.

In this work, we managed a more comprehensive approach towards the discrepency improvement of RANS calculation on an airfoil RAE2822. Flow characteristics information is used to improve the accuracy of numerical calculation of RANS. The next section introduces the numerical approach and the third part follows the method of constructing a data-augmented turbulence model which is based on the discrete adjoint method. The fourth section gives the result and analysis toward the discrepency and correction.

2.NUMERICAL METHOD

There are several widely-used RANS turbulence models, such as the one-equation models Spalart-Allmaras, two-equation model k-omega SST and some other sophiscated models. The construction of turbulence models is based on dimentional analysis, and provide the closure terms of high order fluctuations in N-S equations. These terms are based on the dimensionaless empirical parameters.

The flow solver is setted on a cell-centred finite volume formulation of the compressible RANS equations on structured grids. The inviscid fluxed are discretized under the three-order MUSCL scheme and combined with steger-warming. LUSGS time-steping method.

A C-type mesh with 305 points in the wrap-around direction and 65 points in the wall-normal direction is applied. The total cell number is approxiamately 24,000. The first layer y^+ is set below unity and a grid vertification test is carried out to make sure the calculation accuracy. In the boundary condition, the flow variables at the farfield are set in the freestream condition and the eddy viscosity use the fully turbulent value at $\nu_{t,\infty}/\nu_\infty = 3$. Boussinesq assumptions are used to close the RANS equation.

The freestream flow conditions correspond to a Mach number of 0.729 and Reynolds number of 6.5 million based on the chord length of 1.0 meter with an 2.31 ° angle of attack. The static pressure was computed based on the specified Reynolds number and Mach number and an assumed value of static temperature. The mesh is showed below in Fig 1.

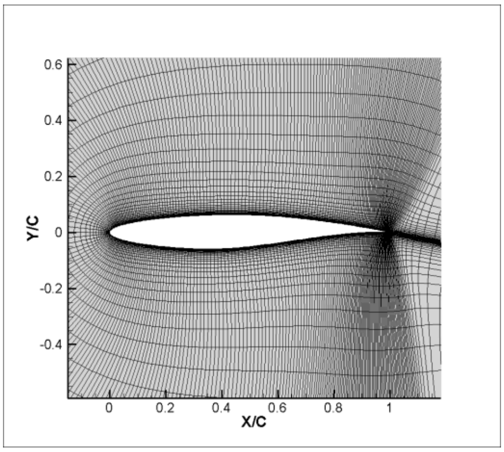


Fig. 1 Mesh of airfoil Rae2822

The Spalart-Allmaras [13] is chosen as the turbulence model in this paper. It can be written as

$$\frac{D\hat{v}}{Dt} = P(\hat{v}, \mathrm{U}) - D\,(\hat{v}, \mathrm{U}) + \mathrm{T}(\hat{v}, \mathrm{U})$$

In which, U represents the Reynolds averaged flow variables and $P(\hat{v}, \mathrm{U})$, $D\,(\hat{v}, \mathrm{U})$ and $\mathrm{T}(\hat{v}, \mathrm{U})$ are the production, destruction and transport terms respectively. They have the formation as,

$$P(\hat{\nu}, \mathrm{U}) = C_{b1}(1 - f_{t2})\hat{S}\hat{\nu}$$

$$\hat{S} = \Omega + \frac{\hat{\nu}}{\kappa^2 d^2} f_{v2}$$

$$D(\hat{\nu}, \mathrm{U}) = c_{w1} f_w (\frac{\hat{\nu}}{d})^2$$

$$T(\hat{\nu}, \mathrm{U}) = \frac{1}{\sigma}[\nabla \cdot \left((\nu + \hat{\nu}) \nabla\hat{\nu}\right) + C_{b2}(\nabla\hat{\nu})^2]$$

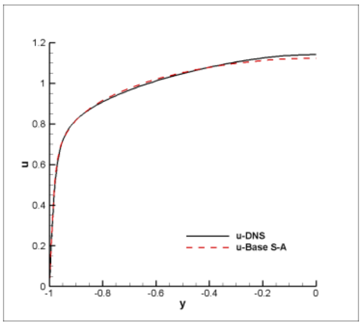
Turbulence eddy viscosity can be gained through:

$$\nu_t = f_{v1}\hat{\nu}$$

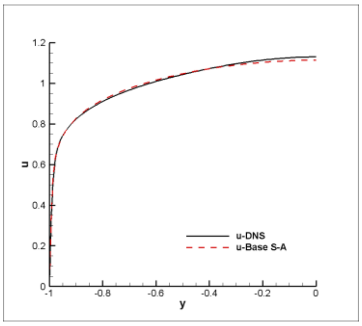
To check the RANS solver, we perform a numerical calculation towards a channel flow under two different Reynolds number. Fig. 2 shows the velocity profile of RANS calculation and DNS database [14]. From the comparison of solution from RANS and DNS, the relative error of velocity and friction coefficient is reasonable which is smaller than 2%.

Table 1 Verification of RANS solver by the relative error of friction coefficient

$C_f(\times 10^{-3})$	DNS	SA-base	Relative error
Re_τ=550	5.8909349	5.9877831	1.64%
Re_τ=1000	5.0954817	5.1198286	0.48%



(a) Re_τ=550



(b) Re_τ=1000

Fig. 2 Comparison of u profile between DNS and S-A turbulence model

3.DATA AUGMENTED MODELING BASED ON ADJOINT METHOD

The coefficients in the turbulence models are decided based on small set of prior flows, so it's hard to construct connection with those important physical characteristic parameters such as local Reynolds number and Mach number, which are changing with different flow conditions or geometry profiles. The major discrepency comes from the turbulence model formation, rather than the option of coefficient. Thus, the conventional methods that adjusting the coefficient have limited effect towards the accuracy of calculation. In this work, a spatially-varying factor $\beta(x)$ is added into the turbulent model equation as a multiply of production term. x refers to each grid point in the domain. The modified model version can be written as,

$$\frac{D\hat{v}}{Dt} = \beta(x) \cdot P(\hat{v}, \mathrm{U}) - D(\hat{v}, \mathrm{U}) + T(\hat{v}, \mathrm{U}) \tag{3.1}$$

The influence of factor $\beta(x)$ is global rather than for production term only, and it can be seen as adding a correction term $\delta(x)$ as $\delta(x) = (\beta(x) - 1) \cdot P(\hat{v}, \mathrm{U})$. Through the introducing of this factor, modified RANS equation can gain a higher accurcy solution. The objective function is stated as:

$$J = \min\{\sum_{j=1}^{N_c}(d_{j,exp} - d_j)^2 + \sum_{j=1}^{N_{cell}}(\beta - \beta_{prior})^2 \} \tag{3.2}$$

Here d represents the flow variables, and $d_{j,exp}$ is the data from wind tunnel experiment [15]. β has a prior value of unity. We choose pressure coefficient for d and thus the objective function can be stated as,

$$J = \min\{\sum_{j=1}^{N_{surface}}\left(Cp_{j,exp} - Cp_j\right)^2 + \sum_{j=1}^{N_{cell}}\left(\beta - \beta_{prior}\right)^2 \} \tag{3.3}$$

The objective function is regularized by a regulation factor λ. It can be introduced to biases the β solution to sit near the initial unity setting. Engineering judgement is required when setting the value of λ. A lower value of λ leads to over-fitting while a higher one may cause fitting failure. We choose a value of 10^{-8} to let the β occupy a small order value in the objective function comparing with the flow variable part.

In order to minimize the objective function, we need to solve out the derivatives of objective function with respect to the design variables. The number of design variables is the same as the grid scale which is very large in an airfoil CFD solver and the conventional finite different method requires large computational resouces. Due to the expansive computational cost, the adjoint method is applied to solve the gradient. The adjoint method is efficient and spend approxiamately only two times of the flow solver's time cost. In the process of solving, the amount of calculation is independent of the number of design variable, and can greatly reduces the calculation time. The adjoint method is based on the control theory of partial differential equation system, and the flow control equation is set as constrains. The aerodynamic design problem is transformed into an optimization problem with specific constrains. In 1927, Jameson [16] first applied adjoint method to aerodynamic design. Since then, continuous adjoint method and discrete adjoint method have been developed. Considering the complexity of code, the discrete adjoint method [17] is adopted in this paper.

$$[\frac{\partial R}{\partial U}]^T\psi = [\frac{\partial J}{\partial U}]^T \tag{3.4}$$

$$\frac{dJ}{d\beta} = \frac{\partial J}{\partial \beta} - \psi^T\frac{\partial R}{\partial \beta} \tag{3.5}$$

Through constructing and solving of adjoint equation in Eq. (3.4), the derivative of the objective function with respect to the design variable $\beta(x)$ can then be obtained from Eq. (3.5). Then, the steepest descent method with fixed step is used to settle the optimization problem. The iteration process is terminated when the objective function attain a steady value. The final set of $\beta(x)$, which is the optimization solution can be embedded into the turbulence model to obtain more accurate calculation results. The coefficient matrix on the left side of the adjoint equation $[\frac{\partial R}{\partial U}]^T$ is a large sparse matrix and this sparse linear system of algebraic equations is solved using fgmres routine, an iterative solver in Math Kernel Library which use the generalized minimal residual method (GMRES) [18].

Accuracy of the adjoint method is verified through a flat plate case. In this case, the coeffient $\beta(x)$ is added into the solver as the way we state. The finite difference method is used by introducing small disturbance to the design variables. The comparison of adjoint method and finite difference method can be seem in fig.3, and the relative error is quite reasonable.

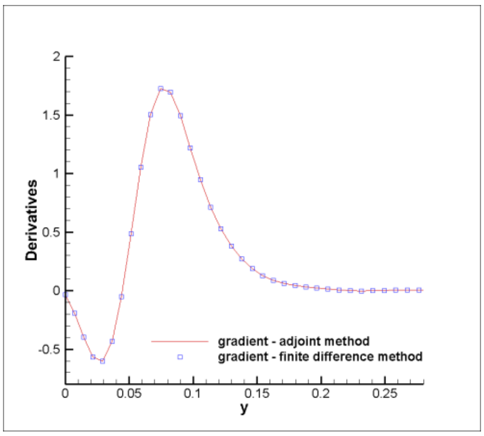


Fig. 3 Verification of adjoint method with the comparison of finite difference method

4. Result and Analysis

The value of λ in objective function is estimated by both the experimental error and the error in base solver and set at 10^{-8}. The result of surface pressure coefficient is shown in fig. 4. The modified S-A model has a higher accuracy in objective function The u velocity field and pressure fields are shown in fig. 5 and fig. 6. The location of shock wave, which is approxiamately recognized by the flattening of the pressure curve, is closer to the experimental data. The lift coefficient, shown in table 2, is improved as well that the absolute relative error decrease from 4.07% to 0.427%.

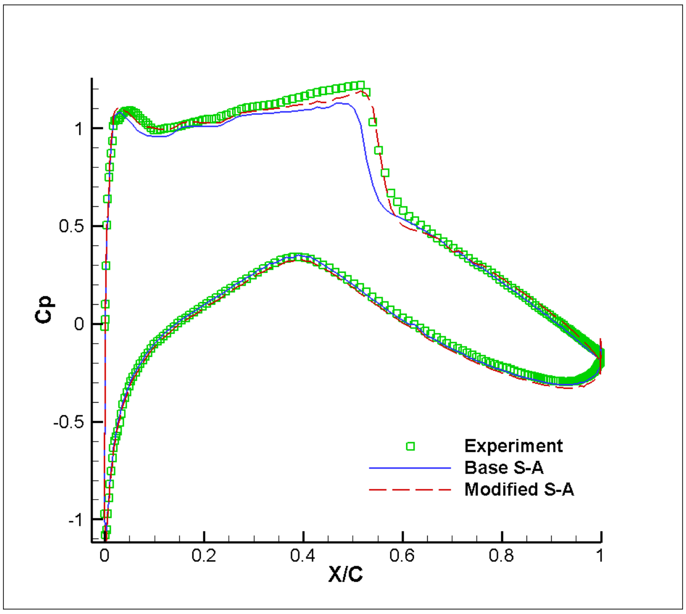
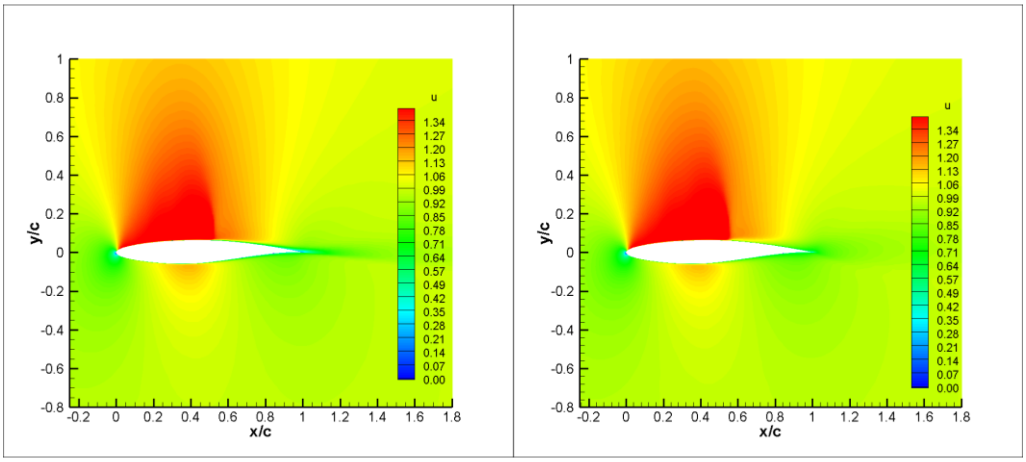
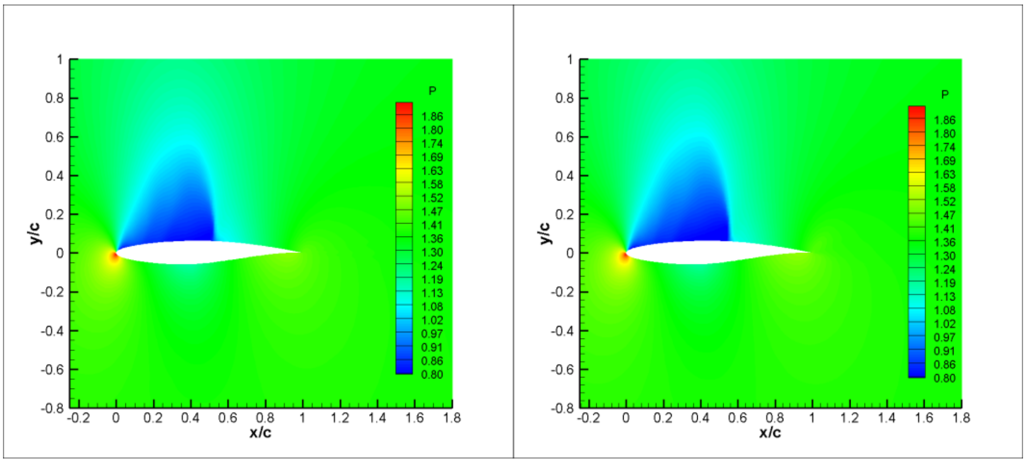


Fig. 4 Surface pressure for the Rae2822 airfoil at Re=6,500,000 and Ma=0.729



(a)Base S-A (b)Modified S-A

Fig. 5 Comparison of velocity fields of airfoil



(a)Base S-A (b)Modified S-A

Fig. 6 Comparison of pressure fields of airfoil

Table 2 Comparison of lift coefficient

	Experiment	Base S-A	Modified S-A
C_L	0.7309	0.70111274	0.727782
Relative error	/	-4.07%	-0.427%

Fig.7 shows the field of correction factor $\beta(x)$, we could see that the regions with significant changes are concentrated near the surface of airfoil and the wake region. The region near the upper and lower airfoil surface is directly related to the pressure coefficient and also dominate the correction field. In the comparison of pressure coefficient, values at X/C=0.55 see a notable change and this is consistent with the peak value in the distribution of correction term.

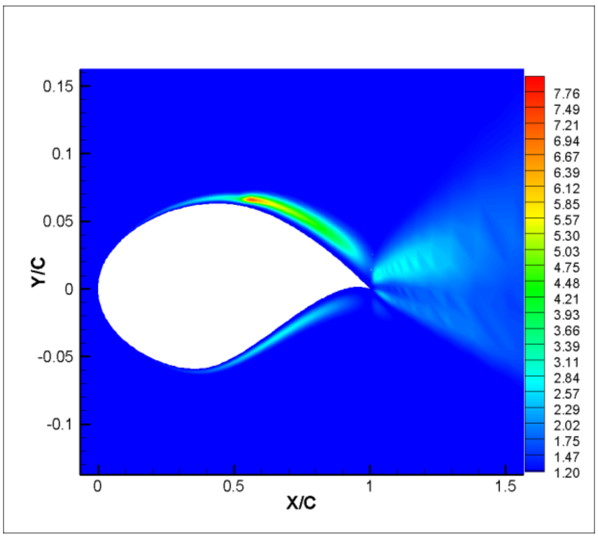


Fig. 7 field of correction factor β

CONCLUSION

The present study proposed a generalized data-augmented turbulence model based on the discrete adjoint formulation which can eliminate the error of turbulence model by adding a correction factor to the producion term in S-A model. After solving the adjoint equation and optimize the distribution of correction factor, the discrepency of origin RANS solution and high fidelity experiment result is corrected. In the process, elements of regulation factor λ and step length affact the correction effect and are designed carefully. A propriate value of regulation factor affact degree of fitting and step length is related to the convergence speed and steadiness. In the result, the accuracy of lift coefficient and pressure coefficient distribution is improved and the distribution of corrective factor is showned.

REFERENCES

[1] Tanno, M., Morimoto, A., Kishiyama, Y., Kawahara, T., Higuchi, K., & Sawahashi, M. (2009). "China, russia establish joint mars exploration team." 2007(9), 1630-1630.

[2] Baldwin, B. S.& Lomax, H.1978 Thin-layer approximation and algebraic model for separated turbulent flows. AIAA Aerospace Sciences Meeting AIAA -78-257.

[3] Pope, S. B. 2000 Turbulent flows. Cambridge University Press.

[4] Mollicone, J., Battista, F., Gualtieri, P., & Casciola, C. 2018 Turbulence dynamics in separated flows: The generalised Kolmogorov equation for inhomogeneous anisotropic conditions. J. Fluid Mech, 841, 1012-1039.

[5] PRANDTL L. Bericht über die entstehung der turbulenz[J]. Z Angew Math Mech, 1925, 5: 136-139.

[6] Schaefer, J., Cary, A., Mani, M., and Spalart, P., "Uncertainty Quantification and Sensitivity Analysis of SA Turbulence Model Coefficients in Two and Three Dimensions," *55th AIAA Aerospace Sciences Meeting, AIAA SciTech Forum*, 2017. URL https://doi.org/10.2514/6.2017-1710.

[7] Schaefer, J., Hosder, S., West, T., Rumsey, C., Carlson, J.-R., and Kleb, W., "Uncertainty Quantification of Turbulence Model Closure Coefficients for Transonic Wall-Bounded Flows," *AIAA Journal*, Vol. 55, No. 1, 2017, pp. 195–213. URL https://doi.org/10.2514/1.J054902.

[8] Parneix, S., D. Laurence, and P. Durbin (1998), A procedure for using DNS databases, Journal of uids engineering, 120 (1), 40{47.3.

[9] H. Xiao, J. L.Wu, J. X.Wang, R. Sun, and C. J. Roy, "Quantifying and reducing model-form uncertainties in Reynolds-averaged Navier–Stokes simulations: A data-driven, physics-informed Bayesian approach," J. Comput. Phys. **324**, 115 (2015)

[10] A. P. Singh and K. Duraisamy, "Using field inversion to quantify functional errors in turbulence closures," Phys. Fluids 28, 045110 (2016).

[11] Ling, J., Jones, R. & Templeton, J. 2016 Machine learning strategies for systems with invariance properties. *J. Comput. Phys*. **318**, 22-35.

[12] Wang, J. X., Wu, J. L. & Xiao, H. 2017 Physics informed machine learning approach for reconstructing Reynolds stress modeling discrepancies based on DNS data. *Phys. Rev. Fluids*. **2**, 1-22.

[13] Spalart, P. R. and Allmaras, S. R., "A One-Equation Turbulence Model for Aerodynamic Flows," **Recherche Aerospatiale**, No. 1, 1994, pp. 5-21.

[14] Myoungkyu Lee and Robert D. Moser "Direct numerical simulation of turbulent channel flow up to Re_tau = 5200", Journal of Fluid Mechanics, 2015, vol. 774, pp. 395-415

[15] Cook, P.H., M.A. McDonald, M.C.P. Firmin, "Aerofoil RAE 2822 - Pressure Distributions, and Boundary Layer and Wake Measurements," *Experimental Data Base for Computer Program Assessment*, AGARD Report AR 138, 1979.

[16] Jameson A. Aerodynamic design via control theory[J]. Journal of Scientific Computing, 1988, 3(3):233-260.

[17] Giles, M., and N. Pierce (2000), An introduction to the adjoint approach to design, Flow, turbulence and combustion, 65 (3-4), 393{415.

[18] Saad, Y., and M. Schultz (1986), GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems, SIAM Journal on scientic and statistical computing, 7 (3), 856-869.