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PDE Constrained Inverse Problems arising from Turbulence Modeling

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Turbulence models, which are a means to fix the closure problem arising from Reynolds averaging of Navier-Stokes equations, are economical stop-gaps but suffer from accuracy issues. Modifying turbulence models by incorporating corrections in their functional form is one approach to improve their accuracy. We estimate correction functionals for the Spalart - Allmaras turbulence model, based on an inverse problem with PDE constraints emphasizing the issue of regularization.

1 Introduction

The numerical simulation of turbulent flows is a challenging problem with several applications in engineering. Simulation strategies include high fidelity methods such as Large Eddy Simulations (LES) or Direct Numerical Simulations (DNS) which resolve the flow field over the bulk of length and time scales but are intractable for large test cases. In contrast, the inexpensive Reynolds Averaged Navier Stokes (RANS) equations, shown below, only resolve the mean flow field $\tilde{u}$

$$\frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial \tilde{u}_i \tilde{u}_j}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \tilde{p}}{\partial x_i} + \nu \frac{\partial \tilde{u}_i}{\partial x_j}\frac{\partial \tilde{u}_i}{\partial x} - \frac{\partial \widetilde{u_i' u_j'}}{\partial x_j}. \tag{1}$$

They are obtained from the Navier Stokes equations by decomposing the flow field u, into the mean $\tilde{u}$ and a fluctuating component u', with $\tilde{u} = \lim_{t\to\infty} \frac{1}{T}\int_0^T u(x,t)\mathrm{d}t$ for a sufficiently large T. Here u_j refers to the j^{th} component of u, ν is the viscosity and ρ is the density. Turbulence models are designed to account for the unknown Reynolds stress term $\widetilde{u_i' u_j'}$.

The most popular approach to turbulence modeling involves the prescription of one or more transport equations with respect to some unknown turbulence quantities. The latter are then related to the Reynolds stresses, typically by means of the Boussinesq approximation. Due to several approximations, the RANS equations with turbulence models approach is prone to errors, especially with respect to integrated quantities such as lift and drag. We consider the problem of modifying the functional form of turbulence models in order to curtail design based accuracy limitations. The estimation of the correction function requires the solution of inverse problems which are naturally ill-posed. We analyze the use of generalized Tikhonov regularization with the inverse problems and consider the problem of optimizing the regularization parameter.

2 Inverse Problems in Turbulence Modeling

We consider the Spalart - Allmaras (SA) turbulence model [1] which introduces the variable $\tilde{\nu}$ called eddy turbulent viscosity via the Boussinesq assumption, governed by the transport equation

$$\frac{\partial \tilde{\nu}}{\partial t} + u_j \frac{\partial \tilde{\nu}}{\partial x_j} = c_{b1}\left(1 - f_{t2}\right)\tilde{S}\tilde{\nu} - \left[c_{w1} f_w - \frac{c_{b1}}{\kappa^2} f_{t2}\right]\frac{\tilde{\nu}^2}{d^2} + \frac{1}{\sigma}\frac{\partial}{\partial x_j}\left(\left(\nu + \tilde{\nu}\right)\frac{\partial \tilde{\nu}}{\partial x_j}\right) + \frac{c_{b2}}{\sigma}\frac{\partial \tilde{\nu}}{\partial x_j}\frac{\partial \tilde{\nu}}{\partial x_j}. \tag{2}$$

This model is modified by introducing a correction functional $\beta(x)$ against its production term $c_{b1}\left(1 - f_{t2}\right)\tilde{S}\tilde{\nu}$. This correction can be estimated by solving inverse problems with respect to a ground truth target functional, such as the lift coefficient C_l measured by experiment. With the linearized governing equations eq. (1) and eq. (2) as constraints, the inverse problem is

$$\min_{\beta} \quad \mathcal{J}(U,\beta) := \frac{1}{2}|C_l^{num} - C_l^{exp}|^2 + \eta r(\beta), \quad \text{s. t.} \quad U^{n+1} = G(U^n, \beta). \tag{3}$$

Here U is the vector of conservative and turbulence variable(s), G is the linear operator of the governing equations and $\eta r(\beta)$ is a regularization term, with respect to the correction β treated as a parameter. The KKT conditions for the constrained problem, based on the Lagrangian $L := \mathcal{J}(U,\beta) + \bar{U}^T(G(U) - U)$ are

$$G(U) - U = 0, \qquad \text{(state eq.)}$$

$$\bar{U} - \frac{\partial J^T}{\partial U} + \frac{\partial G^T}{\partial U}\bar{U} = 0, \qquad \text{(adjoint eq.)}$$

$$\frac{\partial J}{\partial \beta} + \left(\frac{\partial G^T}{\partial \beta} - \frac{\partial U^T}{\partial \beta}\right)\bar{U} = 0. \qquad \text{(design eq.)}$$

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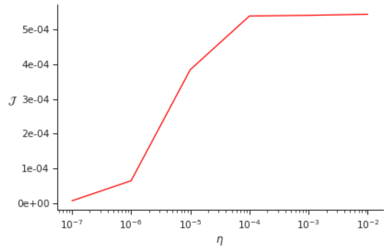
The discrete adjoint framework of algorithmic differentiation [3] is used to solve the adjoint equation in an iterative scheme which follows the solution of the state equation. Subsequently the gradient of the objective function with respect to β is calculated according to the design equation. The inverse problems eq. (3) are then solved using the limited memory version of the BFGS algorithm.

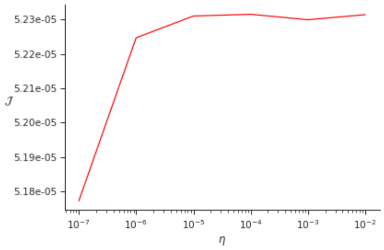
The SA model is well calibrated for aerospace applications and is represented by the unit parameter vector $\beta_{SA} \equiv \mathbf{1}$. The solution of the inverse problem can be biased to approximate the SA model closely if we consider the $\mathcal{L}^2$ norm of the deviation of the parameter β from the usual SA turbulence model, as the regularization. This represents a generalized Tikhonov regularization $r(\beta) = \sum_{j=1}^{p}(\beta_j - 1)^2$. The typical choice for the regularization parameter η is an inflection point of the loss function $\mathcal{J}$. A simple strategy to find the inflection point is to use a brute-force search, which is employed here. A significant drawback is that this search has to be repeated each time the flow conditions or test case is changed.

3 Results

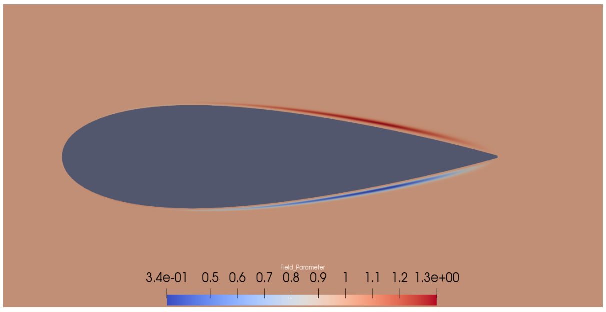
We solve the inverse problems for two different test cases in the open source computational fluid dynamics suite SU2 [4]. The first test case is the NACA 0021 airfoil at angle of attack 0 degrees, Reynolds number 1.5×10^6 and Mach number 0.2. The second test case is the S809 airfoil also at angle of attack 0 degrees, Reynolds number 2×10^6 and Mach number 0.1. Part (a) and (b) of fig. 1 show the objective function value with respect to several different values of the regularization parameter η.



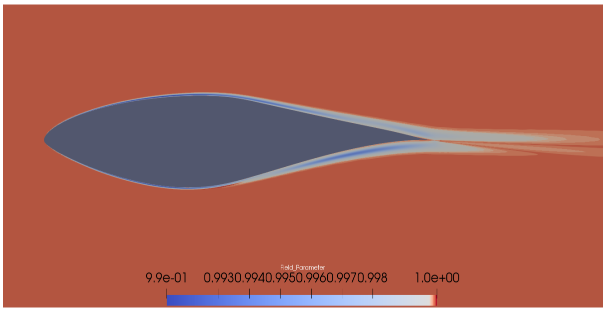
(a) NACA0021: Objective function with respect to parameter η



(b) S809: Objective function with respect to parameter η



(c) Correction function NACA 0021, $\eta = 10^{-6}$



(d) Correction function S809, $\eta = 10^{-6}$

Fig. 1: Correction terms obtained from inverse design and machine learning.

The physical significance of the correction functional is important in order to ensure that non-physical solutions are not obtained due to the correction. The validity of the correction may, for instance, be ascertained using other independent measurements from high fidelity simulations or experiment. The solution of the inverse problem is specific to the particular test case as can be seen in fig. 1. In order to generalize the correction to newer test cases, rather than repeat the inverse design process, a machine learning framework can be established using data obtained from such inverse problems [5].

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