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Uncertainty estimation in large eddy simulations of realistic hypersonic flows

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14. ABSTRACT
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Uncertainty estimation in large eddy simulations of realistic hypersonic flows

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Summary

The main objective of this project has been to develop a systematic and computationally affordable method to estimate the uncertainty in the results of turbulence-resolving simulations, particularly large eddy simulations (LES), of hypersonic flows. The work centered on the development of a method to compute the approximate sensitivity of engineering quantities-of-interest with respect to a large range of uncertain parameters, including insufficiently known boundary or initial conditions, unknown geometrical deviations between the physical and computational models, insufficiently fine computational grids, and inaccurate physics-models. The significance of the work is that it constitutes an important and necessary step towards enabling the use of LES in critical decision making, since the level of confidence in a decision (e.g., "does this design produce sufficiently low drag?") is directly tied to the level of uncertainty in the underlying prediction.

The secondary objective of this project has been to further our understanding of how the near-wall region of turbulent wall-bounded flows is modified by changes in the Mach number and the wall temperature, and specifically to develop improved theoretical models for how the mean velocity profile scales with those changes. This type of near-wall scaling theory is directly used when estimating the wall friction and wall heat transfer in turbulent boundary layers, either in wall-models for LES or in engineering-type friction estimation methods.

The work has been a close collaboration with Sergio Pirozzoli from the University of Rome (he had a companion grant from EOARD, with PM Douglas Smith), with weekly meetings throughout the whole project.

1 Accomplishments

The accomplishments for the two main objectives of the project are described in sections 1.1 and 1.2, respectively.

1.1 Uncertainty estimation in large eddy simulations

The general idea in this work is to estimate the uncertainty in any output quantity-of-interest (QoI) J by the "error-propagation formula"

$$\sigma_J \approx \sqrt{\sum_{i,j=1}^{n} \frac{\partial J}{\partial a_i} \frac{\partial J}{\partial a_j} \Sigma_{ij}}\,,$$

where σ_J is the standard deviation (as a measure of the uncertainty) in the output J (e.g., lift, drag, p'_{rms} over some region, etc), a_i is a vector of n uncertain input parameters (e.g., Mach number, angle-of-attack, turbulence level, etc), Σ_{ij} is the co-variance matrix of the input uncertainties, and $\partial J/\partial a_i$ is the sensitivity or sensitivity gradient. This approach to uncertainty estimation requires a user to use expert knowledge to: (i) decide which parameters are uncertain (and thus define the a_i vector), and then (ii) prescribe values for the co-variance matrix Σ_{ij} that reflect the magnitude and correlations of those input uncertainties.

The technical challenge, and the core objective of this work, is to compute the sensitivity $\partial J/\partial a_i$. Due to the chaotic nature of LES and DNS, there exists no method to compute $\partial J/\partial a_i$ in an accurate yet computationally affordable way for cases with many uncertain parameters. The central research hypothesis of this work is that we can compute a sufficiently accurate approximate sensitivity using the following multi-fidelity approach:

1. Compute a single LES (or DNS, or DES) at the nominal condition and use this as the best estimate of the QoI J;
2. Solve an inference problem for the effective eddy viscosity ν_t field that is consistent with the nominal LES solution, and also the effective thermal diffusivity κ_t;
3. Define a linearized problem for infinitesimal changes in the mean LES solution, using the inferred eddy viscosity, that can be solved affordably in order to find the sensitivity $\partial J/\partial a_i$.

1.1.1 Inferring an effective eddy viscosity from LES or DNS data

After computing the single LES or DNS, we have the mean velocity field U_i and the resolved Reynolds stress tensor field $R_{ij} = \overline{u'_i u'_j}$ (we ignore density variations here for simpler notation). The eddy viscosity hypothesis is that

$$R_{ij} - \frac{R_{kk}}{3}\delta_{ij} \approx -2\nu_t \left(S_{ij} - \frac{S_{kk}}{3}\delta_{ij} \right)\,, \tag{1}$$

where

$$S_{ij} = \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right)$$

is the rate-of-strain tensor and ν_t is the eddy viscosity. The eddy viscosity hypothesis (1) relates the deviatoric (trace-free) Reynolds stress and rate-of-strain tensors; these are labeled with superscript "dev" in the following (i.e., $R_{ij}^{\mathrm{dev}} = R_{ij} - (R_{kk}/3)\delta_{ij}$). We can thus define the error in the eddy viscosity hypothesis (1) as

$$E_{ij} = R_{ij}^{\mathrm{dev}} + 2\nu_t S_{ij}^{\mathrm{dev}}\,. \tag{2}$$

The simplest way to infer the effective ν_t field is to minimize this error in a least squares sense, which leads to

$$\nu_{t,\mathrm{M1}} = \frac{-R_{ij}^{\mathrm{dev}} S_{ij}^{\mathrm{dev}}}{2 S_{ij}^{\mathrm{dev}} S_{ij}^{\mathrm{dev}}} \,, \tag{3}$$

where the "M1" refers to "method 1". This is trivial to compute, but has two potential problems. First, in practice this will produce a rather noisy field due to a lack of perfect averaging, which can create problems in the linearized adjoint solver. Secondly, and more fundamentally, minimizing the error in the modeled Reynolds stress is neither necessary nor sufficient in order to produce a maximally accurate RANS representation. The reason is that the mean momentum equation senses the divergence of the Reynolds stress tensor; thus one could add any divergence-free tensor field to R_{ij} without affecting the resulting RANS solution. All commonly used eddy viscosity RANS models utilize this fact, in the sense that they all knowingly produce very poor predictions of the normal stress components in boundary layer flows – the model developers knew that these produce essentially zero divergence in such flows, and thus knowingly neglected them.

Returning to the present work, the solution is to instead minimize the divergence of the error E_{ij}, i.e., to minimize a cost functional

$$\mathcal{J} = \iiint \frac{\partial E_{ij}}{\partial x_j} \frac{\partial E_{ik}}{\partial x_k} dV \,,$$

where the integral is taken over the full computational domain. This is a calculus-of-variations problem, for which the solution is the so-called Euler-Lagrange equation

$$\frac{\partial}{\partial x_j} \left(S_{kj}^{\mathrm{dev}} S_{ki}^{\mathrm{dev}} \frac{\partial \nu_t}{\partial x_i} \right) + S_{ij}^{\mathrm{dev}} \frac{\partial^2 S_{jk}^{\mathrm{dev}}}{\partial x_i \partial x_k} \, \nu_t = -\frac{1}{2} \frac{\partial^2 R_{jk}^{\mathrm{dev}}}{\partial x_i \partial x_k} S_{ij}^{\mathrm{dev}} \,, \tag{4}$$

which is an elliptic PDE with anisotropic "diffusion". The solution to this equation is termed $\nu_{t,\mathrm{M2}}$, i.e., the "M2" or "method 2" estimate.

The work during years 1 and 2 of this project were largely spent on developing a solver for Eqn. (4). The PI underestimated the challenge involved, mainly brought on by the extreme anisotropy of the "diffusion" in this PDE which makes the standard linear solvers we initially tried unable to find a solution. We therefore had to go back to basics and carefully implement and experiment with more robust numerical methods and solution algorithms. One part of the solution has been to enforce a degree of smoothness on the inferred ν_t field, which helps numerical convergence but also makes perfect sense from an inference point-of-view: we know that the effective ν_t field should be smooth. The smoothness is enforced by augmenting the cost functional to be

$$\mathcal{J}_{\mathrm{augmented}} = \iiint \left[\frac{\partial E_{ij}}{\partial x_j} \frac{\partial E_{ik}}{\partial x_k} + \lambda \frac{\partial \nu_t}{\partial x_i} \frac{\partial \nu_t}{\partial x_i} \right] dV \,,$$

which leads to a penalization of large gradients of ν_t. In terms of the PDE, this adds an isotropic "diffusion" of strength λ (the weight in the cost functional) which helps stabilize and regularize the problem.

The method is tested for a supersonic turbulent boundary layer with a non-adiabatic (heated wall) in Figs. 1 and 2, using DNS data from [1]. We emphasize that there is no "truth" data, so one cannot really discuss the differences as errors. Having said that, the M2 estimate should be closer to the unknown truth by virtue of minimizing the effect on the mean momentum equation rather than relying on the more heuristic idea of minimizing the difference in the stress. Given that, there are clear differences between the M1 and M2 results, thus suggesting that there is value in thinking deeply about how to infer these effective transport properties from DNS and LES data.

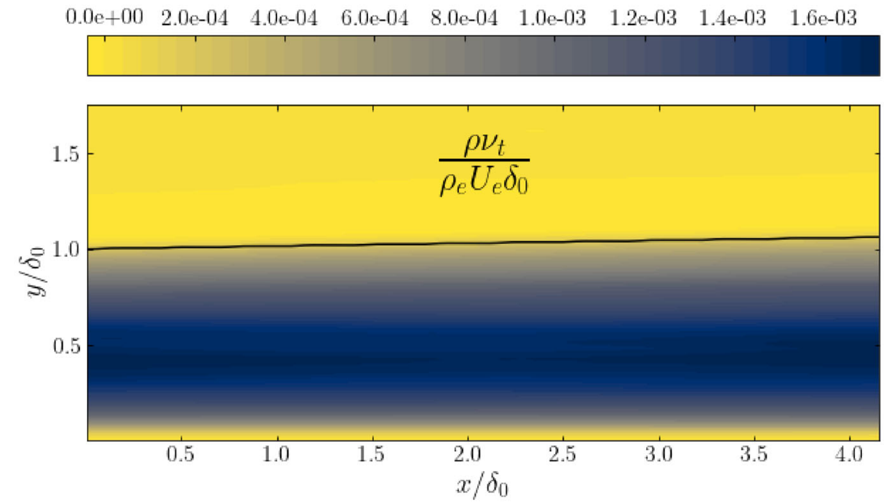

Figure 1: Inferred eddy viscosity from DNS data of a Mach 2.3 boundary layer with a heated wall from the solution to the PDE derived in this work (M2, Eqn. 4). Note how the inferred ν_t follows the growth of the boundary layer, as visualized by the boundary layer edge in the solid line.

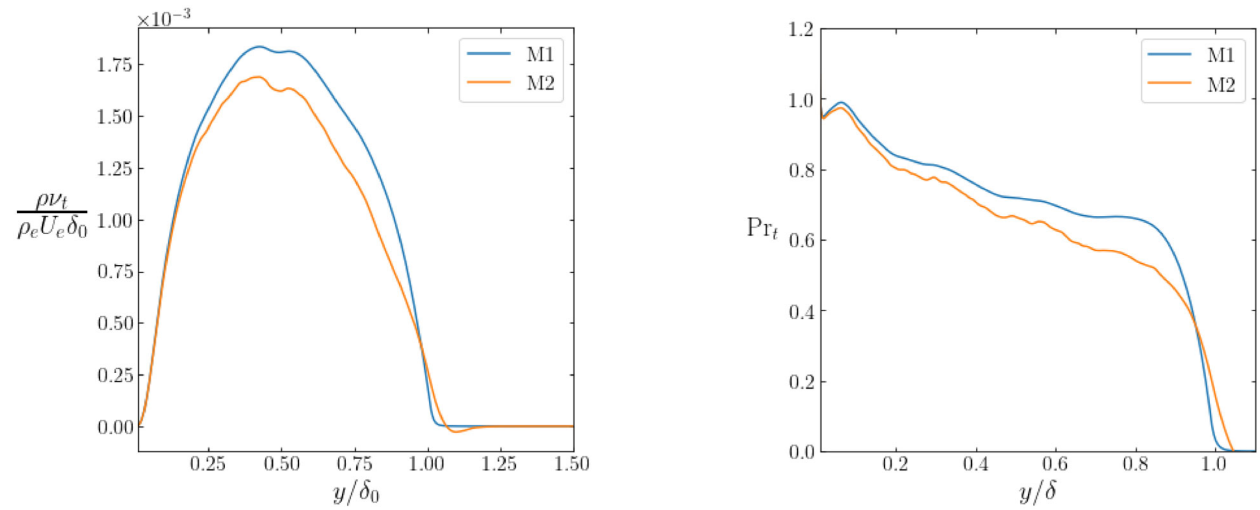

Figure 2: Inferred eddy viscosity (left) and turbulent Prandtl number (right) from DNS data of a Mach 2.3 boundary layer with a heated wall, comparing the local least-squares estimate (M1, Eqn. 3) with the solution to the PDE derived in this work (M2, Eqn. 4).

1.1.2 A RANS problem constrained to exactly reproduce the LES

The process is described here for the incompressible equations for simpler notation. In that context, the RANS equations with the Spalart-Allmaras (S-A) model would be solved for the mean velocity field U_i and the modified eddy diffusivity field $\tilde{\nu}$ that is used in the S-A model. The full RANS equations (with the S-A model) can then be written compactly as

$$\mathcal{M}\left(U_i, \tilde{\nu}; a\right) = 0\,, \tag{5}$$

where a is a problem parameter for which we are interested in the sensitivity of the solution; e.g., a could be the Mach number, the wall temperature, etc.

Now consider a large eddy simulation of the same problem at the same problem parameter a; this would produce a mean velocity field U_i^{LES} that is different from the RANS solution. In addition, we could use the techniques described in section 1.1.1 to compute the inferred effective eddy viscosity field, from which the inferred S-A diffusivity field $\tilde{\nu}^{\mathrm{LES}}$ could be computed. The combination of $(U_i^{\mathrm{LES}}, \tilde{\nu}^{\mathrm{LES}})$ would *not* satisfy the RANS equation (5) due to imperfect inference and imperfect averaging. However, we can define a constrained RANS problem as

$$\mathcal{M}\left(U_i, \tilde{\nu}; a\right) - \mathcal{M}\left(U_i^{\mathrm{LES}}, \tilde{\nu}^{\mathrm{LES}}; a\right) = 0\,. \tag{6}$$

In other words, we evaluate the full set of RANS equations for the known LES solution, and then subtract this residual from the RANS equations. This constrained problem has the solution $(U_i^{\mathrm{LES}}, \tilde{\nu}^{\mathrm{LES}})$ for parameter value a, by construction. In other words, this RANS problem has been modified to exactly reproduce the LES solution at the nominal condition. We can then use this constrained RANS problem to explore the parameter space, either by sampling, parametric studies, or by linearizing the problem.

The definition of this constrained RANS problem is the mathematical heart of the whole proposed method.

1.1.3 Sensitivity estimation for a shock/boundary-layer interaction

The proposed method to estimate sensitivity is tested for a shock/boundary-layer interaction (SBLI) at Mach 2.3 with a moderately cold wall ($T_w/T_r = 0.5$), where we want to estimate how changes in the wall temperature T_w and the shock angle β affect the mean solution.

We first perform an LES at the nominal condition and compute the mean fields and the Reynolds stresses. This simulation is done on a grid with about 200M grid points, and thus represents a significant computational cost. We then compute the inferred eddy viscosity and thermal diffusivity using the method in section 1.1.1 (at negligible cost), and form the constrained RANS problem as described in section 1.1.2. We then solve the constrained RANS problem for several different values of the perturbed wall temperature T_w and the shock angle β, and compute the sensitivity of the solution by finite differencing in the parameter. For example, the sensitivity of the mean velocity field is estimated as

$$\frac{\partial U_i}{\partial T_w} \approx \frac{U_i(T_w + \Delta T_w) - U_i(T_w)}{\Delta T_w}\,.$$

It should be emphasized that this constrained RANS problem is *much* cheaper than the LES: in the present work, we use grids with about 0.5M grid points since the RANS equations are actually defined in two dimensions for this problem. The total cost of the sensitivity estimation process is thus 1-2 orders of magnitude lower than the cost of the LES itself.

To assess the accuracy of the results, we compute the “true” sensitivity by running LES at multiple perturbed conditions and using the same finite differencing concept. This process is very expensive as it requires multiple LES cases; it is done here only to provide reference data for the accuracy assessment.

The results are shown in Fig. 3. For comparison, the results using stand-alone RANS (the current best-practice) are included. The figure should be interpreted as: which of the red (current state-of-the-art) or green (proposed method) lines is closest to the blue one (the “truth”)? While the proposed method certainly is not perfect, it is measurably better than the sensitivity estimated from stand-alone RANS simulations. The improvement is greatest for the sensitivity of the Stanton number with respect to the wall temperature ($\partial c_h/\partial T_w$). For the other quantities, the main improvement is an improved prediction of the spatial extent of the sensitive region.

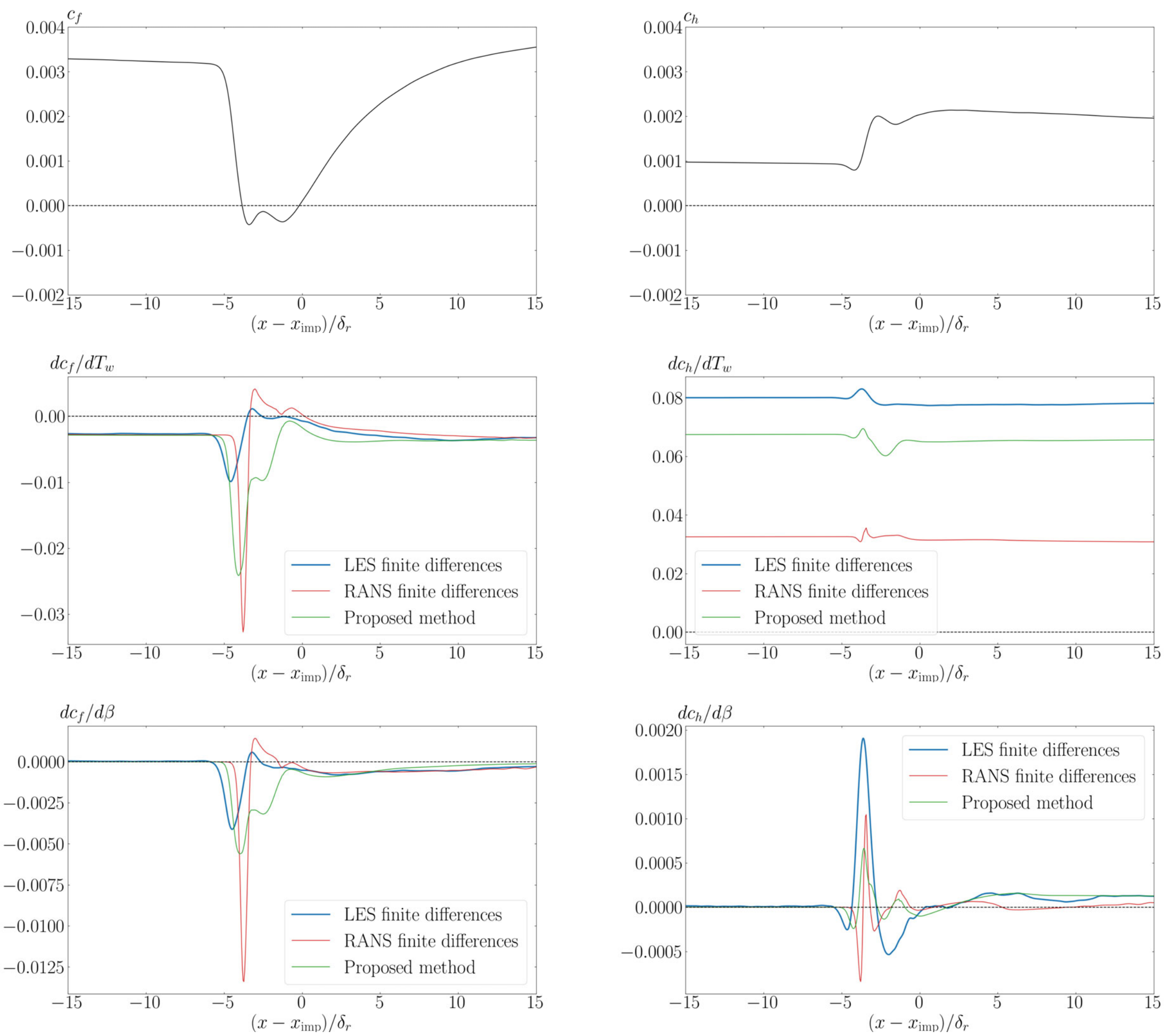

Figure 3: Assessment of sensitivity estimation method for a shock/boundary-layer interaction problem, showing the nominal friction (c_f) and heat transfer (c_h) coefficients (top row) and the sensitivity of those quantities to changes in the wall temperature T_w (second row) and the shock angle β (third row). The blue line is the "truth", the green line is the proposed method, the red line is the current state-of-the-art when using stand-alone RANS.

We emphasize that the computational cost is identical between the proposed method and the stand-alone RANS simulations (excluding the nominal LES case, which is not meant for sensitivity estimation). We therefore view this as a successful proof-of-concept of the proposed method. There is clearly a need to improve the accuracy, for which the most plausible avenue is to increase the fidelity of the RANS model: the Spalart-Allmaras model used here was chosen for simplicity rather than maximal accuracy.

1.2 Near-wall scaling for non-adiabatic hypersonic turbulent boundary layers

Compressible turbulent boundary layers have non-uniform density and viscosity profiles which cause the mean velocity profile to disagree with the classic (and supposedly universal) log-law. A very important question is therefore how these density and viscosity non-uniformities affect the near-wall behavior of the turbulent boundary layer. By "near-wall scaling" we here mean the mean velocity profile, the Reynolds stresses, and the scaling of the wall-distance in the inner part of the turbulent boundary layer.

The pioneering work in this area was by Van Driest [2] who used dimensional reasoning to derive how the mean velocity gradient should scale in the presence of a non-uniform density field in the log-layer. This was later put into the form of an integral transformation of the mean velocity by Danberg [3], now known as the famous "Van Driest transformation". While this scaling works well for adiabatic boundary layers of arbitrary Mach numbers, it fails for strongly non-adiabatic (especially cooled) ones. In earlier work we derived an alternative near-wall scaling theory [4] based on two different physics-based arguments. One was the dimensional analysis by Van Driest, the other was an argument about how the momentum equation for nearly parallel flows should be satisfied in both the real and transformed states. The resulting transformation (which affects both the mean velocity and the wall-distance coordinate; in fact, the perhaps biggest contribution of that work was to make the argument that there can only be one scaling of the wall-distance for all types of quantities) works very well for internal flows (like channels), well for strongly cooled boundary layers at modest Mach numbers, and increasingly poorly for higher Mach numbers and closer to adiabatic walls.

We made progress on three fronts of this problem during this project: (i) we developed a novel partially data-driven velocity transformation (section 1.2.1); (ii) we developed a more discerning test of theories based on the idea of "unrealistic" fluids (section 1.2.2); and (iii) we developed an improved method for engineering friction and heat transfer estimation based on the most recent theories (section 1.2.3).

1.2.1 A data-driven, physics-constrained, velocity transformation

We derived yet another transformation by combining one physics-based argument (the momentum conservation argument by Trettel and Larsson [4]) with a brute force calibration of the remaining free parameters [5]. More specifically, we restricted ourselves to transformations of the original u and y to the transformed (and supposedly universal) U and Y of the form

$$\begin{aligned} Y &= \int_0^y \left(\frac{\rho}{\rho_w}\right)^b \left(\frac{\mu}{\mu_w}\right)^{-a} dy\,, \\ U &= \int_0^u \left(\frac{\rho}{\rho_w}\right)^b \left(\frac{\mu}{\mu_w}\right)^{1-a} du\,, \end{aligned} \tag{7}$$

where a and b are free parameters. Note that Eqns. (7) satisfy the momentum conservation argument by construction. We then used some DNS data from the literature plus some additional cases created specifically for this purpose to calibrate the a and b constants. The important step was to create cases with "artificial" fluids with highly non-standard viscosity-temperature relationships in order to untangle the effects of density- and viscosity-variations. The calibration process produced $a \approx 3/2$ and $b \approx 1/2$ as the best values. The resulting transformation was then validated on other DNS cases from the literature, a sample of which is shown in Fig. 4.

This new transformation works rather well, in fact better than any other transformation across the full Mach number range and wall temperature range. In that sense this was a strong success. However, the fact that we did not derive (from physics) the right values of the a and b parameters but instead used calibration reduces the value of this work, in this PI's opinion. This type of "data-driven" approach, where physics insight is supplanted by use of data and optimization methods, produces results without the insight. The PI realizes that "data-driven" and the associated "machine learning" are very popular these days, but is very much not on that bandwagon. Nevertheless, there

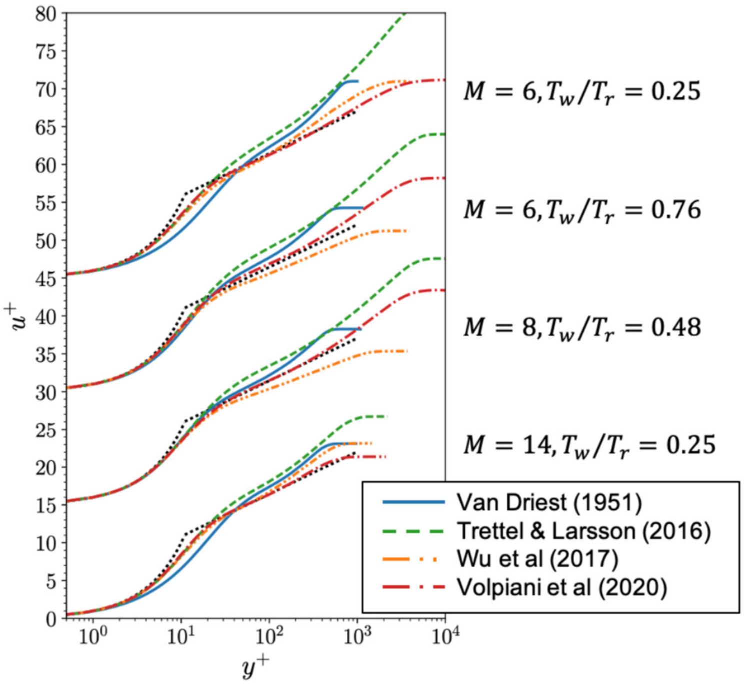

Figure 4: Assessment of different near-wall scaling theories on four different hypersonic boundary layers (DNS data from Zhang *et al.* [6]).

is value in this new transformation, specifically that: (1) we can now think of physics-based reasons for why those specific a and b values are the right ones; and (2) the fact that the calibration is unable to produce perfect collapse implies that at least one of the three physical assumptions made in its derivation is not fully correct: (i) the assumed integral form of the transformations in Eqn. (7) may be too restrictive; (ii) the assumption of power-law dependencies of the density and viscosity in the integral kernels may be insufficiently accurate; and/or (iii) the assumed importance of the momentum conservation argument by Trettel and Larsson [4] may be incorrect.

1.2.2 A strong test for near-wall theories: unrealistic fluids

As multiple different theories for how near-wall turbulence is affected by compressible flow effects have been proposed over the last decade, the question of how to differentiate between theories has become more nuanced. If two theories provide roughly equal accuracy for the limited validation data sets available, does that mean that those two theories are equally valid and meaningful? In our view the answer is "no", primarily due to the very limited nature of the available validation data, as it covers only a small part of the full parameter space. One new idea that we pursued in this project is that we can significantly expand the parameter space of validation data by considering direct numerical simulations (DNS) of turbulent boundary layers in "unrealistic" fluids, where "unrealistic" means fluids that do not exist on Earth. The basic rationale is that a valid theory for near-wall turbulence should be applicable to *all* fluids, not just those present on Earth. This turns out to be a very strong and highly discriminating test of theories.

The easiest way to create an "unrealistic" fluid is to change the viscosity-temperature relationship. Supersonic turbulent boundary layers have a non-uniform mean temperature distribution across the boundary layer, which creates a non-uniform density distribution through the equation of state (the pressure is approximately uniform). Most gases have a viscosity μ that increases with

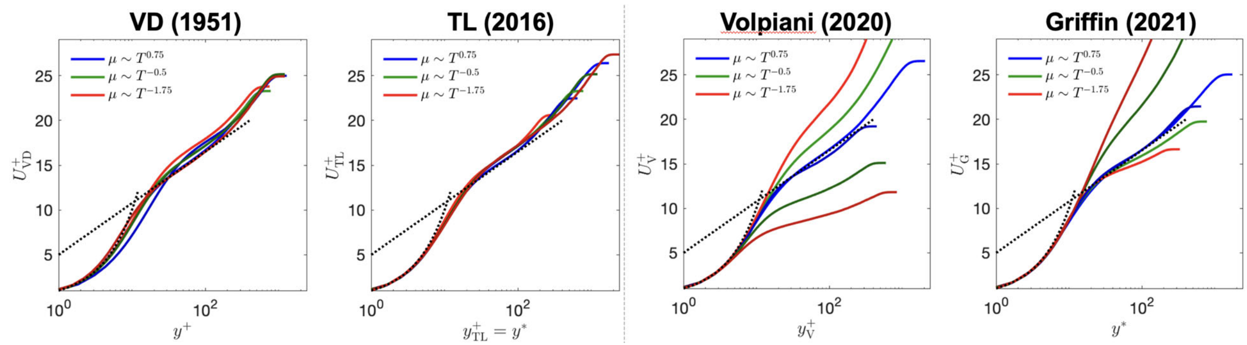

Figure 5: Tests of near-wall scalings using "unrealistic" fluids, where the viscosity-temperature relationship has been altered compared to standard air. Showing the theories/transformations of Van Driest [2], Trettel and Larsson [4], Volpiani et al [5], and Griffin et al [8].

temperature T; e.g., air under typical conditions has $\mu \sim T^{0.75}$ or so, with the exact value of the exponent depending on the temperature range. In the present work we also run simulations of boundary layers with $\mu \sim T^{-0.5}$ and $\mu \sim T^{-1.75}$. The reason for these specific choices can be found in the viscous length scale l_v, which (approximately) describes the distance over which viscous effects are felt. This viscous length scale is defined as $l_v = \mu/\sqrt{\rho \tau_w} \sim \mu \sqrt{T}$. The two "unrealistic" fluids used here therefore correspond to either a spatially uniform viscous length scale (for $\mu \sim T^{-0.5}$) or a viscous length scale that varies inversely compared to that of air (for $\mu \sim T^{-1.75}$).

After running the DNS cases, the data was used in multiple different theories/transformations with the results shown in Fig. 5. To interpret the figure, note that a perfect transformation would collapse all colored curves (supersonic cases) onto the black curve (the incompressible one). The results are pretty stunning in clarity: the most recent theories of Volpiani et al [5] and Griffin et al [8] are clearly incorrect (note: the PI was a co-author of the former paper, so this is self-criticism). In contrast, the classic Van Driest theory and the one by Trettel and Larsson behave well under these conditions, albeit still not providing perfect collapse.

This type of result is very helpful, as it shows that the theory baked into the VD and TL transformations is mostly correct while the theory that is the basis for the Griffin et al transformation is not. It also shows the limitations of data-driven work: these cases go outside the calibration (or "training") range of the method, and then all bets are off.

1.2.3 A modular method for friction and heat transfer estimation

The development of near-wall scaling theories is a fundamental pursuit, but it has direct impact on engineering estimation processes. In practical engineering scenarios, it is highly useful to be able to estimate the friction and heat transfer coefficients in a cheap manner. Specifically, one wants to estimate the c_f and c_h from knowledge of only the Reynolds number Re, the Mach number M, the wall thermal condition as quantified by the wall-to-recovery temperature ratio T_w/T_r, and the fluid properties (equation of state, viscosity-temperature relationship). The current state-of-the-art is the the so-called "Van Driest II" method [9], which is based on an analytical inverse of the Van Driest transformation and assumptions about the relationship between velocity and temperature.

In this project we developed an improved method for engineering estimation that is based on the most recent theories available. The method is numerical in nature since there is no known inverse of the most recent velocity transformations; however, it can be run on a laptop in fractions of a second. The method and complete validation is described in Kumar and Larsson [10], with the key validation result shown in Fig. 6. The proposed method reduces the maximum error (among all

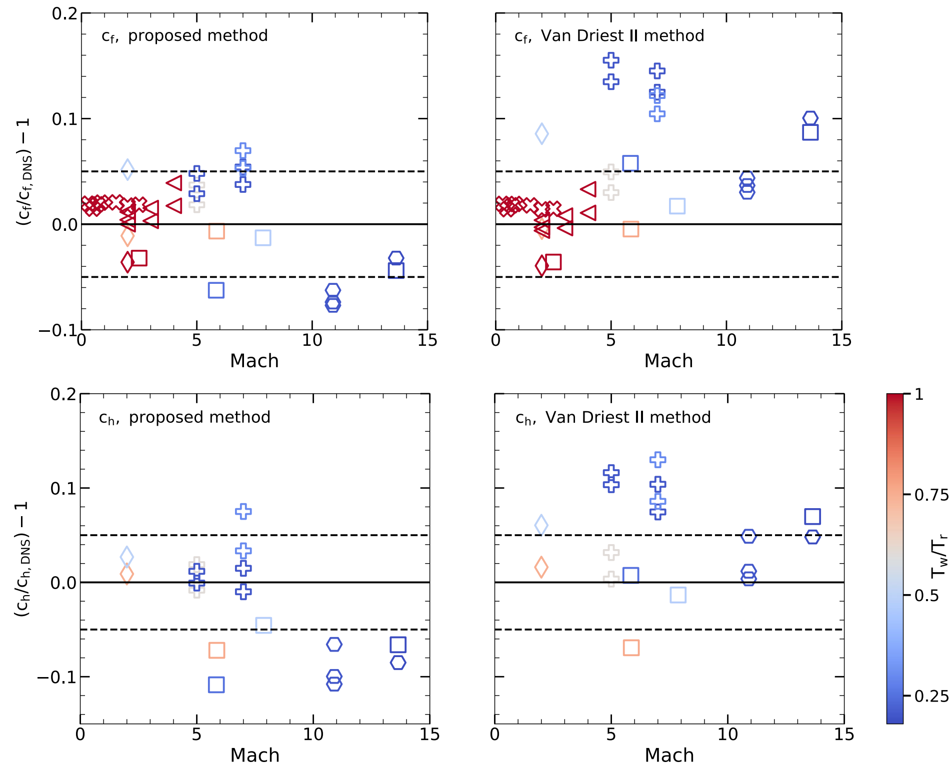

Figure 6: Validation of the newly developed engineering estimation method [10], showing the error between the estimated value of c_f (top row) and c_h (bottom row) and the true value from DNS. Comparing the proposed method (left) with the Van Driest II method (right).

validation cases) from 16% to 8% in the friction coefficient c_f, and from 13% to 11% in the heat transfer coefficient c_h. The main improvement occurs for cases with Mach numbers above 5 and highly cooled walls, i.e., exactly the flow regime of interest in hypersonic aerodynamics.

2 Impacts

The method for engineering estimation of wall friction and heat transfer could be used in conceptual design of new hypersonic vehicles immediately, and the Python code is available for download from the PI's website. The fact that this method reduces the error in the predicted friction by half at hypersonic conditions means that the conceptual design can be more accurate and thus will have less need for later corrections. This estimation tool is expected to make a direct impact on hypersonic vehicle assessment and design.

3 Changes

Nothing to report.

4 Updates

Nothing to report.

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