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NASA Symposium on Turbulence Modeling: Roadblocks, and the Potential for Machine Learning

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Langley Research Center, Hampton, Virginia

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Abstract

A three-day symposium sponsored by NASA was held in July 2022 in Suffolk, Virginia on the subject of Turbulence Modeling: Roadblocks, and the Potential for Machine Learning. This meeting brought together over 80 experts from academia, government, and industry to discuss critical issues for Reynolds-averaged Navier-Stokes turbulence and transition models, as well as to evaluate the results from a collaborative testing challenge based on data-driven methods and machine learning technology. This report puts this symposium in context with an earlier similar meeting and summarizes many of the questions, discussions, and conclusions that arose from it. Next steps are suggested.

1 Introduction and overview of the symposium

In computational fluid dynamics (CFD), turbulence modeling within the context of the Reynolds-averaged Navier-Stokes (RANS) equations remains one of the greatest sources of uncertainty. Over the last half century, countless turbulence models and model variants have been developed in an effort to yield useful CFD predictions for basic and applied fluid flows in the aerospace field. Although often very accurate for attached equilibrium flows, these models, ranging from simple algebraic to seven-equation transport, have often failed (to various degrees) for other classes of flows. Consistently accurate predictions of separated flows have been particularly elusive; and these play a key role in many aerospace flowfields of interest such as conditions near maximum lift and stall.

In this landscape, many vehicle designers and analysts often make due with the existing RANS shortcomings because of its relatively low cost, and attempt to manage risk by assigning more uncertainty to CFD results involving (for example) separated flow. However, for complex configurations containing many different flow features mixed together, managing such risk can be very difficult. Because of this, many CFD practitioners have been recently moving toward more frequent use of costly scale-resolving simulations (SRS), in which turbulence is resolved rather than modeled (except at the finest scales). Although current computational capability – and thus the reach of SRS – is greater than it has ever been, these types of simulations are still out of reach for many users and applications, especially at high Reynolds numbers. SRS also have had considerably less time than RANS to mature. There are currently many different SRS methodologies and practices in use. As a result, it is unlikely, at the current time, that two different SRS codes would be able to yield completely consistent results for a given problem.

Thus, the CFD world finds itself at a kind of crossroad. RANS computations are inexpensive but can be inaccurate in many situations. SRS are more accurate in general, but they are much more expensive to run and still require a considerable level of expertise to execute correctly. And some configurations that are handled quite successfully with RANS (such as the attached boundary layer over a full-sized wing) would be prohibitively expensive for current SRS. Which is the best path to follow? Most people today feel that RANS will be useful and necessary for many decades to come. But because of the trend away from RANS toward SRS, funding and training in RANS turbulence modeling has all but disappeared, leaving RANS apparently stagnating in terms of development or acquisition of new ideas.

In 2017, a three-day turbulence modeling symposium was held in Ann Arbor, Michigan. The purpose of this meeting was to discuss the state of the art in turbulence modeling, including emerging ideas. Questions surrounding its future were also addressed. A particular question asked was whether RANS modeling has already reached an 'ultimate barrier,' preventing further significant progress. As documented in Duraisamy et al. [1], that symposium also initiated discussions regarding if and how machine learning (ML)[1] methods might be best applied to RANS turbulence models.

[1]Throughout this paper, ML is used to refer to machine learning and its associated automated tools used to leverage data toward making predictions or decisions. ML is nowadays the most common moniker for this field of research and development. However, the term 'data-driven modeling' may more accurately reflect the overarching processes in play, with

Regarding model improvements, one of the main conclusions to emerge was that, because of the reduced levels of RANS research, better coordinated efforts are required going forward. Opinions were varied as to whether RANS modeling can make progress or not. Some felt that we have not come close to reaching an ultimate barrier yet and more research into RANS modeling is called for; others felt that modeling accuracy will likely never improve by much, so more effort should go into SRS and quantifying uncertainties in models. Regarding the use of ML for improving turbulence models, early data-driven modeling trials indicated that improvements to RANS are possible, but very difficult to generalize. Some specific recommendations were made: (1) establish benchmark problems and practices specifically for the purpose of developing and evaluating data-driven turbulence models; (2) strive to maintain a balance between RANS research and SRS research by devising a recommended turbulence modeling research roadmap that ties into CFD Vision 2030 [2]; (3) decide on a common site for a direct numerical simulation (DNS) and large eddy simulation (LES) dataset repository that can be used for RANS model improvements; (4) better catalog and track experimental datasets; and (5) hold follow-up symposia.

As will be described in this paper, a first attempt was made to establish benchmark problems in the current symposium: it was named a 'Collaborative Testing Challenge for Data-Driven Turbulence Models.' But regarding the other recommendations above, only the last (holding follow-up symposia) has been done. However, for item (3), scattered individual efforts to house high-resolution datasets have been occurring spontaneously in many places throughout the world. To name a few, these include the European Union Horizon HiFi-TURB project[2], which is creating a database wiki knowledge base (still under development at the time of this writing), a JAXA DNS database website[3], the Johns Hopkins Turbulence Databases website[4], and the TurBase website[5].

In 2021, a symposium (sponsored by the University of Michigan) related to the one held in 2017 was held virtually on Model-Consistent Data-Driven Turbulence Modeling [3]. Its focus was primarily on machine-learning-augmented turbulence modeling, with emphasis on promoting consistency between the training and prediction environments. Talks were grouped into several categories of techniques: evolutionary/symbolic, field inversion, integrated inference and learning, and emerging.

The current in-person symposium, titled 'Turbulence Modeling: Roadblocks, and the Potential for Machine Learning', was conceived as a follow-on to the 2017 symposium. It was originally scheduled to take place in early 2021, but was delayed due to COVID restrictions until July 2022. The symposium had two themes[6]: (1) identification of critical issues for RANS models, as well as possible ways forward; and (2) a Collaborative Testing Challenge for data-driven RANS models. The latter theme arose because of one of the recommendations from the 2017 symposium, as described above.

The three-day symposium was held in Suffolk, VA at the Lockheed Martin Center of Innovation. It included 25 participant talks, five keynote talks, and three panel discussions. The full list of talks is provided in the Appendix. Total attendance was just over 80 people, with roughly 45% from academia, 45% from national or military labs, and 10% from industry. There was representation from the U.S., Australia, Germany, The Netherlands, Belgium, Japan, France, and South Korea.

The purpose of this paper is to distill key points from the symposium, with an overarching goal of continuing to chart a possible roadmap or recommended path forward for data-driven improvements to turbulence models. No effort is made to summarize the contents of individual talks[7]; the slides from these are all available on the symposium's website [4], along with (for a limited time) videos of

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the actual 'machine learning' making up only a part of it. In this paper, the two terms are often used interchangeably.

[2]https://www.numeca.com/hifiturb-horizon2020-project, cited 10/4/2022.

[3]https://jaxa-dns-database.jaxa.jp, cited 10/4/2022.

[4]https://turbulence.pha.jhu.edu, cited 10/4/2022.

[5]https://turbase.cineca.it, cited 10/4/2022.

[6]Although not its primary focus, the 2022 symposium was also held in honor of Philippe R. Spalart's contributions to the turbulence modeling field. Dr. Spalart was also involved in the symposium's organization, and he delivered two keynote talks and led the RANS panel discussion.

[7]The individual talks were mostly on specific topics related to recent research regarding benchmark data and RANS-model development, ML-based or otherwise.

the keynote presentations and the panel discussions. The keynote talks and panel discussions were highly useful for their introduction and overview of the issues surrounding ML applied to RANS modeling.

2 State of RANS modeling, and role of Machine Learning

As mentioned earlier, one of the main questions addressed in 2017 was whether RANS models have already hit an *ultimate barrier*, implying that further improvements are not possible. We learned that there are many different opinions about this question, and no clear way at this point to decide who is right. Regardless of the answer, RANS closures have experienced very few deep changes over the past two decades; any advances tend to be relatively minor adjustments to existing models. So today, the fundamental question seems to be: *Since turbulence modeling progress via the human brain appears to be mostly incremental, can this impasse be overcome through the use of data-driven/machine-learning technologies?* This question will take center stage in what follows.

The following subsections summarize the keynote talks, statements from the RANS-modeling panel, and the ensuing discussions.

2.1 Spalart keynotes

One of P. R. Spalart's goals in his first keynote talk (*'An old-fashioned framework for machine learning in turbulence modeling'*) was to provide guidance, from a turbulence modeler's point of view, for ML practitioners, including describing pitfalls, needs, and constraints when creating or improving turbulence models. He began with background comments, acknowledging the challenges associated with transmitting and receiving 'turbulence culture,' described as 'a mix of rigor and intuition, which takes years to acquire.' One should also understand that using ML for RANS-model development involves 'billions of turbulence facts' (say, from multiple DNS) but not 'billions of model constants,' and in this sense differs from other applications of ML. Spalart stressed that, to date, no general-purpose ML-based model had even been produced, much less found to be successful.

Specific advice for the ML community was then offered:

- A general-purpose model that 'tries to do everything' is needed (specialized zonal models are of limited value, since industrial practice is to solve problems with multiple flow features conflated in a single solution). Perfection is not required, but stability and sensible results are.
- The simple flat-plate/zero-pressure-gradient boundary layer should not be sacrificed; any new model must yield an accurate skin friction coefficient for this flow, since it is one area of clear success for turbulence theory, and relevant to so many engineering applications.
- Any model should respect Galilean invariance and independence of the direction of the axes.
- Any model should strive to have robustness in general, and attend in particular to its effect on turbulence (i) in a mature vortex (i.e., does not create spurious vorticity of opposite sign), and (ii) on the edge of a turbulent region, ensuring the vortical/irrotational interface propagates away from, not into, the turbulence. (The latter can be assessed by applying the model to an exact-solution test problem in which only the diffusion terms are active.)
- Avoid acceleration and pressure-gradient dependence in models, since these have no direct effect on the turbulence, and can be introduced to or removed from the equations by a simple change of reference frame.

Spalart ended his first keynote talk with a few reflections on ML. He pointed out the difference between a model *correction* for a single flow – which can be instructive for a human modeler – and a model per se. The overarching role of ML was also questioned: 'will [ML] be the *architect* [of a new model] or only in charge of *subtasks* [such as adjusting constants]?'[8] Spalart ended his first presentation by confessing his lack of any promising, new ideas about the way forward for developing ML-based RANS improvements, while remaining open to the possibility that they may exist.

This talk prompted a number of comments. As in the 2017 symposium, some discussion took place regarding the generalized k-ω (GEKO) RANS model (currently unpublished in its details) devised by Florian Menter. With GEKO, the user is given control over adjustable parameters that change various specific behaviors of the model. For example, the amount of separation, the jet width, or the strength of corner vortices can be controlled by the user. The main issue with this type of tuning is that the user must know in advance what type of flow phenomena are present in the particular problem being simulated. It was brought up that it may be difficult to make use of GEKO for unknown problems or problems with many different flow phenomena present together, although the ANSYS Fluent software apparently allows for the parameters to be field variables that can take different values in different regions. A key feature of GEKO is that it is constrained to give the same flat-plate boundary layer with any setting. In essence, then, GEKO is designed to improve turbulence modeling capability via users' expert knowledge regarding the problem under consideration, without allowing the user to adversely affect the standard boundary layer. As described below – and consistent with Spalart's second bullet point, above – this 'do no harm' goal is also advocated for data-driven turbulence modeling, for which ML would replace the user.

Spalart's second keynote talk (*'Conjectures of a generalized law of the wall and a structural limitation for classical turbulence models',* given at the end of the ML/RANS-model material on the third day) dealt with the practical implications of the fundamental differences between actual/measured RANS quantities in wall-bounded turbulence and the same quantities predicted by classical turbulence models. (His aim was to give 'specific reasons to not keep tweaking [model] constants' – a view also articulated during the RANS-modeling panel discussion.) The point is that these 'classical models' (which include all common one-point closures, such as k-ε, k-ω, Spalart-Allmaras (SA) [with and without the quadratic constitutive relation (QCR) correction], and Reynolds Stress Transport (RST)) can be shown to satisfy a Generalized Law of the Wall (GLW) that is *not* in general satisfied by actual data[9]. Turbulence scientists have been aware of this problem[10] since the 1970s, and it exists outside turbulence modeling because the GLW under other names is the 'natural' extension of the reasoning that succeeds for the mean velocity, but is not a theory from first principles. Top experts have proposed theories such as 'inactive motions' (defined as motions that do not contribute to the divergence of the Reynolds stress, which is what enters the momentum equation[11]) and the Attached-Eddy Hypothesis to explain the conflict and make fairly successful quantitative predictions. These theories involve the wall-bounded flow as a whole, as opposed to a one-point representation. Unfortunately, neither of these theories have led to functional corrections to the one-point classical models; this could be blamed on lack of effort, or it could be a manifestation of the limitation.

The challenge posed by this 'structural limitation' could well be especially severe for ML-based enhancements of RANS models because of the step up in the expectations, fed by the enthusiasm for ML and by the growing availability of very detailed datasets, most of them from DNS. The DNS training ground is very confined in terms of flow type and Reynolds number; the community is investing considerable effort into correcting this[12]. Unless it is explicitly ruled out, the ML correction

[8] After reflecting on all the presentations and comments, the present authors' conclusion is that most if not all participants appeared to subscribe to the latter option. This view was exemplified by Paul Durbin, who proposed it is 'better to use ML for model *enhancements* [of existing models, rather than creation of new ones].'

[9] Spalart conceded that the GLW *may* appear in the data at 'enormous' Reynolds numbers, beyond any yet measured.

[10] In the discussion that followed this keynote, Durbin raised the finding from DeGraaff and Eaton's zero-pressure-gradient boundary-layer experiments [5], that the Reynolds stresses require *two* velocity scales to exhibit similarity, as another indication of the fundamental inconsistency between classical theory and reality.

[11] Girimaji reminded the gathering that motions that are 'inactive' with regard to momentum transport cannot be assumed to have no effect on the transfer of other quantities, such as heat and scalar fluxes.

[12] See Charles Hirsch's keynote below.

may attempt to break through the limitation by inappropriate modifications (such as alterations to viscous corrections outside the viscous region) that cannot be expected to have any general validity. A similar danger exists for strategies using net outputs on the body's surface (such as lift, pressure, or skin-friction distributions) but no field information in their cost functions, in that it is very difficult to detect compensations of errors. Spalart concluded by asking if there are 'nonclassical but CFD-friendly [e.g., local] models waiting to be created [by ML]?'.

2.2 Huang: *The anchor points of turbulence modeling*

In George Huang's keynote talk, he raised the following questions regarding data-driven methods:

- Can ML be made less dependent on the geometry of the training flows?
- Can ML-based corrections be rationally extended to high Reynolds numbers (since DNS and LES only offer low-Reynolds-number training data)?
- Can ML retain its 'memory' (i.e., build on previous success, rather than having to start from scratch)?
- To what extent can ML capture actual flow physics?
- Can ML satisfy asymptotic behaviors of benchmark flows?

As an example of the issue raised by the flow-physics question, it is well known that most RANS models severely underpredict the magnitude of the turbulent shear stress in the separated shear layer off of smooth bodies (Huang refers to the higher-than-modeled magnitude of the actual shear stress as the 'slingshot effect'). As a results, most RANS models tend to predict flow reattachment too far downstream, and delay subsequent boundary-layer recovery. An important challenge for ML methods is to allow RANS models to accurately predict this effect, without adversely affecting predictions of other flow phenomena where RANS already works well.

Regarding Huang's last question, it was noted there are a few benchmark flows often used by turbulence modelers to calibrate models, such as the standard zero-pressure-gradient flat plate boundary layer, and its log-law velocity profile. Huang called these benchmark flows 'anchor points,' and suggested that any work in ML-based turbulence modeling needs to ensure they are always satisfied. (This reinforces a point raised by Spalart in his first keynote.) Huang also issued a 'Grand Challenge' for ML-based models to independently recreate the log law 'from scratch,' solely from experimental or numerical data, with no a priori assumptions.

2.3 RANS-modeling panel

The RANS panel consisted of Paul Batten (Metacomp Technologies), Paul Durbin (Iowa State University), Charles Hirsch (Cadence-Belgium), and Brian Smith (Lockheed-Martin). In addition, P. R. Spalart (moderator) collected opinions in advance from Florian Menter (ANSYS) and Michael Strelets (NTS), both of whom were unable to attend. The RANS panelists were asked to address three questions:

- Is there stagnation in RANS turbulence modeling?
- Does it matter?
- What activities, including ML, can cause a breakthrough?

The answer to the first question varied. A few of the panelists said 'yes' there is stagnation and a few said 'no.' However, among those who said no, all agreed that RANS progress tends to be incremental. Given enough time, it could see major improvements[13]. On the other hand, instead of using the word 'stagnation,' Durbin preferred to describe the situation as 'business as usual' for this field – given its necessarily ad hoc, heuristic, evolutionary nature.[14] But whether they were optimistic or pessimistic regarding the rate of current progress, all panelist agreed RANS models leave much room for improvement. Unfortunately, the fact that SRS methods are becoming more affordable seems to be slowing progress. As more industries (the automotive industry is one) recognize the advantages in accuracy, and increased affordability, of SRS, and adopt it to a greater degree, less funding, training, and research is going into RANS methods. However, the use of SRS for many aerospace design applications, with their very high Reynolds numbers, is still too expensive, particularly when many thousands of CFD runs are required as part of a design process. Many industries will therefore need to rely on RANS for the foreseeable future.

For this reason, the panelists generally agreed that RANS models still *do* matter. They will always serve as a lower-cost capability. RANS modeling should be thought of as an engineering tool, with inherent limitations built into its derivation. For example, one should never count on RANS models to work well for cases with significant complexity, either in terms of geometry or flow features, for regions far outside the parameter space for which they were developed (which typically only spans two-dimensional, equilibrium benchmarks). And RANS models are also important because they are an essential component of many SRS methodologies (e.g., in the near-wall region) or even for use in precursor computations, defining appropriate upstream and boundary regions for SRS.

Regarding the possibility of ML (or any other activity) potentially causing a breakthrough for RANS models, the answer among the panelists was generally rather negative. While most of the panelists agreed that data-driven methods offer the potential for some improvements, they typically gave ML little hope for producing a groundbreaking leap forward, particularly while remaining in the conventional ('classical') RANS modeling framework. (Recall Spalart's discussion of the structural limitations of classical models, described above.) Furthermore, turbulence statistics can exhibit strong bifurcations, and behavior in different bifurcation branches can be very different. Because ML cannot extrapolate reliably, this means that training data are needed from any and all bifurcation branches. This is an extraordinarily tall order. One idea expressed was that ML could potentially put a framework around zonal model usage, by automating it. With this, various 'tunings' of a RANS model (such as GEKO) could be trained to be automatically applied zonally in different flowfield regions, as appropriate. It was also suggested that the reliability of RANS results might be significantly enhanced if the focus was placed not on absolute values but on differences between cases.

The idea was put forth that brute-force data crunching may not be sufficient for turbulence modeling; appropriate intelligence/wisdom needs to be 'baked into' the ML. We need to know the sensitivities of the dependencies (for example, fixing the Reynolds-stress anisotropy is not useful if it is not important for a given problem). Furthermore, we may still be clinging to old, unnecessary RANS paradigms. Even exact results (such as the tensor-invariant, basis-function expansion for the Reynolds-stress anisotropy; see Sandberg's keynote talk) are subject to the fundamental restrictions introduced by the one-point nature of the underlying constitutive relationship (e.g., dependence of the local Reynolds stress upon on the local Reynolds-averaged velocity gradient). One must pay attention to both the 'magnitude' and the 'shape' of turbulence. (Recall Spalart's lecture on the structural limitations of classical models.) Perhaps we need to step back and ask: if we did not already have RANS and instead were starting with ML, what would we do to create predictions for turbulent flows?

[13]In Menter's memorable words, 'RANS turbulence modeling is like a turtle – it does not move when you watch it, but over time it can cover significant distances.'

[14]Durbin compared the time between landmark developments in Quantum Mechanics (from Planck's in 1897, to Schrödinger's in 1925) to that between Boussinesq's eddy-viscosity hypothesis and Prandtl's mixing length – also in, respectively, 1897 and 1925.

3 Applications of Machine Learning to RANS modeling

This section contains summaries of two keynote talks describing specific ML strategies applied to RANS modeling, the outcomes of a panel discussion on ML, and miscellaneous comments and observations.

3.1 Sandberg: *Recent evolution of Gene-Expression Programming for developing turbulence models*

Richard Sandberg described improvements to RANS models applied to turbomachinery[15], using Gene Expression Programming (GEP). The improvements are in the form of a Reynolds-stress tensor model, written as an expansion of powers of the velocity-gradient tensor U_{ij}, nondimensionalized by a local, scalar turbulence timescale, and weighted by scalar functions ('diffusion coefficients') that depend solely upon the invariants I_k of U_{ij}. (Under the assumption the local Reynolds stresses depend only upon local diffusion coefficients and local/one-point components of the velocity gradient, this tensor expansion is finite and exact, due to the Cayley-Hamilton theorem; see Pope [6]. However, in spite of the tensor nature of the resulting diffusion coefficients, because of the limitations inherent in these assumptions of dependency, the exactness of the tensor expansion is not sufficient in and of itself to produce an exact RANS closure.) The I_k dependence of the diffusion functions is determined via GEP, with the resulting Reynolds stress correction altering the RANS equation, and (in the most recent applications) the production terms in the k-ω transport equations. The GEP strategy was chosen because it provides a robust, 'plug-and-play' symbolic regression, which produces models that are interpretable, analytic functions. GEP is an evolutionary, 'survival of the fittest' algorithm, based on the mapping between symbols (representing both mathematical operations and independent variables) and equations [7]. Each entry from a population of such symbols is assessed, by comparison with training data (from experiments or simulations), with the resulting 'fittest' model being the training outcome. (Because assessment of the candidates involves a RANS CFD solution, any unstable or unsuitable model functions are automatically eliminated.) Extensions to unsteady RANS and LES were discussed, as was multiobjective training, based on simultaneous improvements to Reynolds-stress and heat-flux predictions.

3.2 Hirsch: *The HiFi-TURB project – Vision and progress of ML-based turbulence modeling*

In his keynote talk, Charles Hirsch described the ERCOFTAC[16] HiFi-Turb project[17]. The central tasks of this EU-funded study are to create an extensive database of high-fidelity solutions (via DNS and WRLES), and to use it to train turbulence models with ML tools. The project includes work packages to improve both explicit algebraic Reynolds-stress models (EARSM) and the pressure-strain model used by RST closures. An important practical issue that has come to light in the EARSM effort is that most existing high-fidelity data are very limited in terms of where various flow properties reside in parameter space. For example, the mean vorticity/strain-rate quantity $r = \Omega^2/(S^2 + \Omega^2)$ is generally very close to 0.5 for most of the flows that have been computed for this exercise. This makes it difficult for ML, because it has to extrapolate in the regions nearer to $r = 0$ and $r = 1$. One way around this may be to create synthetic data (from EARSM), to augment the existing LES and DNS data. In their ML strategy, they have found that guidance from physical knowledge is required. An unintelligent approach (using data blindly) inevitably fails.

[15] Turbomachinery applications tend to involve lower Reynolds numbers than many aerodynamic applications, so that transition is often a crucial aspect. But even without transition, these applications are challenging for RANS models due to their complex interacting flow phenomena, nonequilibrium, three-dimensional boundary-layer separation, vortex shedding, wake distortion, and the mix of stochastic and deterministic unsteadiness, such as from wake/boundary-layer interactions.

[16] 'European Research Community On Flow, Turbulence And Combustion.'

[17] 'High-Fidelity LES/DNS data for innovative Turbulence models.'

Hirsch also discussed the path forward for SRS in industry. He believes that high-order methods combined with GPU technology may soon be game changers, allowing for far more accurate SRS at a significantly lower cost. If this is the case, then SRS may assume a more prominent position in industrial practice sooner than previously believed, supplanting RANS and lessening the critical need for improved RANS models in the near term.

3.3 Machine-Learning panel

We now turn to the ML panel, which consisted of Andrew Banko (West Point), Paola Cinnella (Sorbonne University), Richard Dwight (TU Delft), Sharath Girimaji (Texas A&M University), and Robert Moser (University of Texas at Austin). Karthik Duraisamy (University of Michigan) served as moderator. The panelists were provided the following topics and ideas to spur discussion:

- Questions:
  - Do we even have the right descriptors to have a chance at succeeding (do we need structure tensors)?
  - How can we rationally isolate/combine the impact of different nonlinear phenomena (e.g., separation, secondary flows, pressure gradients, curvature) in model construction?
  - How to identify the right set of (hard and soft) constraints that should be satisfied? (cannot be under- or overconstrained)
  - How to coordinate high-fidelity simulations and experiments with model development?
  - How can the community work together more cohesively?
  - What should be the role of NASA?
- General suggestions:
  - Set goals and expectations: address the dissonance between what researchers in data-driven turbulence modeling have actually been doing and what the community thought they have been doing
  - Do not oversell what can be done with ML
  - Try to use common terminology
  - Show bad results (things that did not work), not just good results
  - The community needs more emphasis on the importance of uncertainty quantification
- ML challenges:
  - Incomplete data
  - Lack of convergence
  - Irrecoverable model discrepancies
  - Lack of identifiability, generalizability, or interpretability
  - Input and output constraints

During the panel discussion, the above questions/ideas were not specifically or consistently addressed. Instead, alongside the prepared panelist remarks, the topics stimulated additional related comments and thoughts, some of which are summarized below. The last two questions above were revisited (although not fully resolved) during the final discussion regarding next steps at the end of the symposium.

There was some pushback regarding the need for a universal (generally applicable) turbulence model. Many people do use special models for specific classes of flows; they want the best possible model for a given application, and perhaps current ML practices can provide that. This may be thought of as 'goal-oriented' RANS modeling. It is more along the lines of coming up with a surrogate model for specific types of flows.

Some discussion took place regarding the uncertainty and usefulness of turbulence models in general. There are several levels of uncertainty in RANS and LES turbulence models. At the highest level, there is uncertainty introduced by ensemble averaging. Fundamentally, this is not recoverable. Then there is uncertainty in the functional and operational representation of Reynolds stresses, such as single-point closures, linear constitutive relations, etc. Next, there is uncertainty in the functional form of the model and model components (e.g., the pressure strain model, the diffusion term). Finally, at the lowest level, there is uncertainty in the model coefficients. In spite of the fact that models are often created under very restrictive assumptions (that formally define a specific range of applicability), in practice they are often used – and are useful – well outside of this. Ultimately, predictive capability is the final arbiter of a model's usefulness. Respecting formal flow physics and achieving engineering goals are often at odds with one another. Most engineers do not care about model derivation or details, they only care about the end result that it produces. A common axiom that was repeated during the symposium is: 'All models are wrong... but some models are useful.'

It was stressed that at the fundamental level, ML is nothing more than statistics and numerical analysis/linear algebra ('curve-fitting' was mentioned), and we have already been using these capabilities for a long time. However, ML tools have advanced the ability to automate these processes and apply them easily and automatically to huge datasets. Unfortunately, dramatic advances in some areas (such as facial recognition) have raised unrealistic expectations of what can be done with ML for RANS models. It needs to be stressed that within the field of turbulence modeling, ML is likely only going to be a small part of the entire process. For example, we likely will need to intelligently preprocess the training data before ML is started. The data also need to be properly weighted, and someone very knowledgeable in turbulence modeling will likely need to carefully curate the data and the training process (act as a 'supervisor').

We appear to be very far away from the goal of having ML yield groundbreaking insights in turbulence models. Some of the biggest roadblocks to generality appear to be (1) nonlocality, and (2) the 'hugeness' of turbulence (its range of scales, its nonlinearity, its complexity, etc.). Related to the latter point is that for some flows the Reynolds average is formed over both nonturbulent/irrotational and turbulent/vortical regions, and the Reynolds stresses contain both deterministic and stochastic unsteadiness.

3.4 Miscellaneous comments

We conclude the Applications of ML to RANS Modeling material with a few observations and suggestions, gleaned from the presentations and discussions over the course of the symposium.

3.4.1 *ML strategies employed during the symposium*

The goals of the researchers working in this field appear to cover a wide range; there are many niches in CFD where turbulence modeling comes into play. For example, some of the goals alluded to during the symposium include: developing a general predictive turbulence model, improving results for a specific (narrow) class of flows, modeling for RANS, modeling for LES, modeling for hybrid approaches, and using ML as a postprocessing step. Ultimately, this broadness of the field could make collaboration more challenging.

Because ML is such a 'hot topic' today, with the field exploding and many researchers crowding into it, advancements in ML software and techniques are occurring at breakneck speeds. All of these emerging ML methods are difficult to stay abreast of. As a result, different researchers rarely employ the same methodologies[18], so repeating, verifying, and learning from others' work can be

[18]Recall the categories used for the 2021 University of Michigan symposium [3]: evolutionary/symbolic, field inversion, integrated inference and learning, and emerging methodologies.

very difficult to achieve.

Various types of 'CFD-driven' ML methods were discussed during the symposium. With these, the training is combined with RANS calculations in some sort of integrated way, so that consistent subsequent performance of the developed RANS model is more likely. In this approach, any ML-based enhancements that yield unstable CFD results would not survive the training process. This idea was also mentioned in Sandberg's keynote talk.

It is well known that ML is very good at performing interpolation, but it extrapolates very poorly. In discussions, 'extrapolation-detection methods' were mentioned. Presumably, these could be useful to try to detect and avoid situations where the ML uses features outside the range over which training has occurred. One speaker showed plots where points were colored in the flowfield according to whether they were interpolated or extrapolated, allowing the user to visualize the regions where the ML was likely to be reasonable versus poor. This brings up the point that millions of control volumes does not necessarily mean millions of useful training points. Typically, it is much less.

3.4.2 *Suggestions*

A recurring issue during the symposium was the challenge associated with – and the critical importance of – deciding which features should be used in the training[19]. Although ML practitioners should resist the temptation to 'throw everything in and see what works,' and to strictly avoid using spurious, unphysical quantities (such as those that violate Galilean and coordinate-system invariance), we expect new and creative thinking on this topic will be needed if ML is to have a profound and long-lasting impact on RANS modeling. Researchers are also reminded of the limitations inherent in the (local, one-point) RANS formalism; the ideal features would circumvent these limitations, while providing viable (stable, efficient) improvements for practical CFD.

Perhaps the most serious criticism regarding current ML-based-RANS-model publications is they tend *not* to provide models that can be used by the RANS-CFD community at large. (This was also brought up by Spalart in his keynote lecture on the old-fashioned framework for machine learning in turbulence modeling.) This resistance to providing full, usable model details may be due to ML-based models being trained only for a single, narrow class of flows. Or it may be because the training process in any research effort can yield many different models or versions of models, with the *process* itself considered as the publishable entity and none of the resulting models complete/thorough enough to be considered 'final' or worth publishing. While this approach is understandable as modelers attempt to 'find their feet,' too often it limits the ability to independently test/evaluate new contributions and thereby collectively make more rapid advances.

Some of the speakers included uncertainty estimates when they showed predictions from their ML-based models. This was seen as a very positive and useful thing, as it provided the audience with a more realistic sense of the model's predictive capability.

The community was asked to consider sharing code, equations, and ML architectures. (This is common practice among computer scientists working in ML.) The possibility of creating common challenge cases, using the same data, was also raised.

The use of a common home website for data-driven turbulence and transition modeling (DDTTM) was also recommended, perhaps as a subpage of the NASA Turbulence Modeling Resource (TMR) website [8]. This site would serve to: (1) keep notes for this community; (2) list useful ML-related papers; (3) curate challenge cases; and (4) post links to high-resolution databases for future training needs.

[19]This challenge was illustrated by Eisfeld's talk, during which it was shown that different flows (in this case boundary layers and mixing layers) require different values for the same model coefficient.

4 Transition modeling and Machine Learning

Three talks and a panel discussion on data-driven transition modeling took place on the afternoon of the third day of the symposium.

The transition-modeling panel consisted of Karthik Duraisamy (University of Michigan) and Heng Xiao (Virginia Tech). Paul Durbin (Iowa State University) served as moderator. The transition panelists were asked to address the following questions:

- Must transition models be based on data correlations?
- Are data-driven methods attractive for transition modeling?
- There is no theory of transition. What does this mean for analysis and modeling of transition in practice?
- Intermittency models suppress eddy viscosity; e^N methods purport to predict transition onset. Should the paradigm be predicting transition or suppressing the turbulence model?

In the discussions, it was noted that determining transition location seems to be amenable to data-driven discovery (as opposed to a need for physics-based methodologies). However, appropriate feature selection is still very difficult (it is more empirical/intuitive). Transition modeling is different from turbulence modeling in that it includes many nonlocal and global parameters. On the plus side, because of the (generally) lower Reynolds numbers for transitional problems of interest, it is more within reach of DNS. (On the other hand, DNS of transition must deal with a wide parameter space of transition-inducing perturbations, such as the size and nature of surface roughness, and the distribution, amplitude, frequency and wavelength of freestream disturbances.) In the ML process, one can use feature space design to try to reduce the amount of extrapolation. For transition, ML can come into play for different models, including linear stability theory, parabolized stability equations, or correlation-based transport partial differential equations (PDEs).

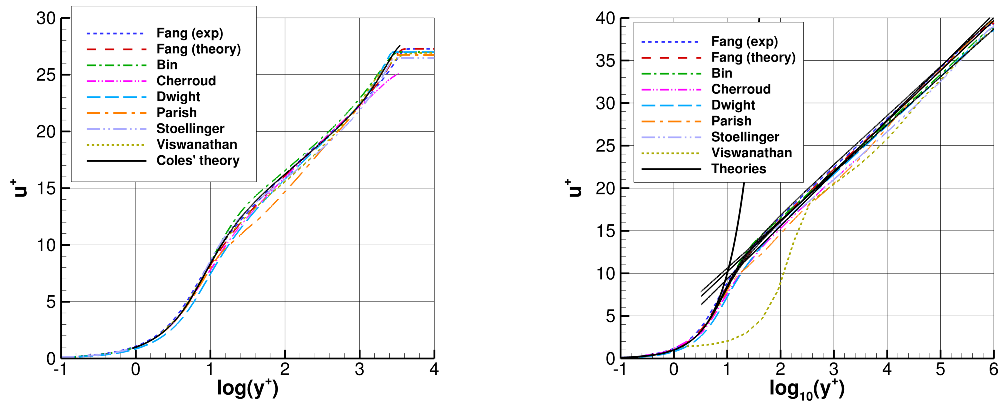
5 The Collaborative Testing Challenge

An important part of the 2022 Symposium was a first-ever challenge for the data-driven turbulence modeling community. As mentioned above, typically in the literature, data-driven methods and machine learning applications have not provided specific models that can be readily used by others. In particular, improvements to models are usually only applicable to cases that are very similar to those they were trained for. And sometimes, data-driven models that are applied well outside of the range of applications they were designed for can yield strange, nonsmooth, or even nonsensical results [9].

The CFD community is seeking improved turbulence models that can be used more generally and confidently in predictive situations. Arguably, this implies the need for a somewhat universal model. At the very least, any new model should ‘do no harm’ to the RANS model’s ability to predict basic flows like the flat plate. The worst thing a model can do is to yield terrible or unexpected results in certain situations, because models often get applied to very complex configurations with many different flow topologies present. In such cases, defaulting to a standard model rather than trying to extrapolate based on machine-learned data would probably be preferable.

The ‘Collaborative Testing Challenge’ was conceived as an integral part of this symposium, with the idea of getting a group of experts to try to achieve data-driven turbulence models that work well across a fairly wide range of simple test cases. Each participant was to apply their best turbulence model scheme (framework) derived from a preferably data-driven approach to a variety of flows specified by the conference organizers. To be a valid entry, the same turbulence model must be applied to each of the following cases (all from the TMR website [8]):

- 2DZP: 2D Zero Pressure Gradient Flat Plate Validation Case



(a) 2DZP case: zero-pressure-gradient flat plate (b) 2DFDC case: high Re fully developed channel

Figure 1. Velocity profiles in inner variables (log law plots).

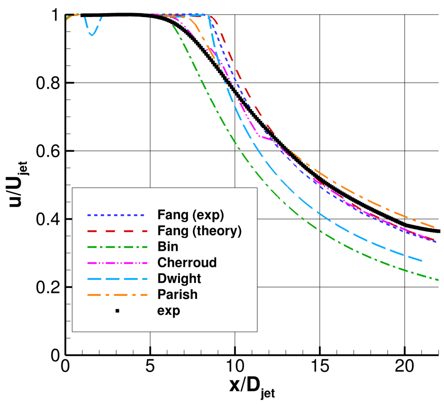
- 2DFDC: 2D Fully Developed Channel Flow at High Reynolds Number Validation Case
- ASJ: Axisymmetric Subsonic Jet
- 2DWMH: 2D NASA Wall-Mounted Hump Separated Flow Validation Case
- 2DN00: 2D NACA 0012 Airfoil Validation Cases (4 separate cases)

Eight participants signed up for the challenge. Seven ended up submitting results (although one of them submitted two sets). A brief summary of each method is given in Table 1. Details about the methods are not provided here, but can be found in the participant talks posted to the symposium's website [4]. A few comparison plots of results are shown here. Complete results can also be found in the Challenge Collective Results presentation posted to the symposium's website [4]. Note that some participants did not complete/submit one or more of the test cases.

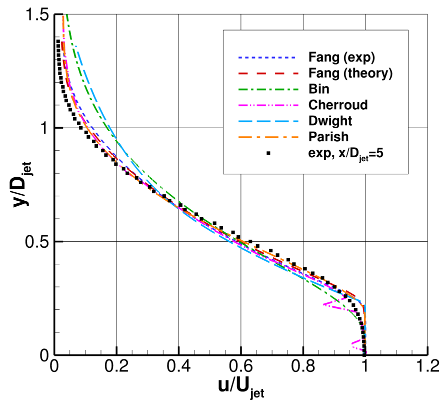
Table 1. Challenge Participants and Brief Summary of Methods.

Participant	Method
Fang (exp)	Gene Expression Programming (GEP) optimized based on experiment
Fang (theory)	GEP optimized based on theory
Bin	Data driven fix of SA model (do no harm... protect law of the wall)
Cherroud	Separately trained EARSM models aggregated
Dwight	Baseline SST model... then trained a classifier model
Parish	Ensemble of Neural Networks (NNs) with training data other than challenge cases
Stoellinger	Human-trained model
Viswanathan	Ground truth: SA model itself
Marepally	Field Inversion Machine Learning (FIML) on SA model (S809 airfoil for training)

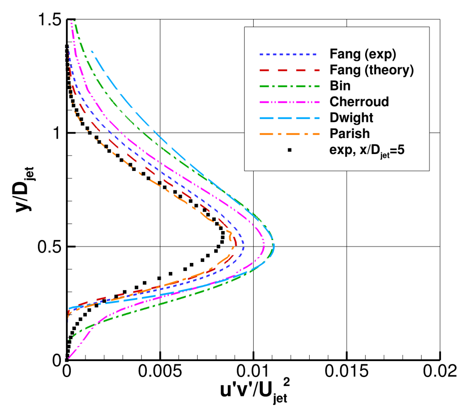
Proper log law behavior was captured reasonably well by most (but not all) participants who submitted results, as noted in Fig. 1(a) and (b) for 2DZP and 2DFDC, respectively. For ASJ (Fig. 2(a)), four of the participants came fairly close to the evolution of the centerline velocity far downstream, but only two were close to predicting the behavior near the start of velocity dropoff



(a) Centerline velocity

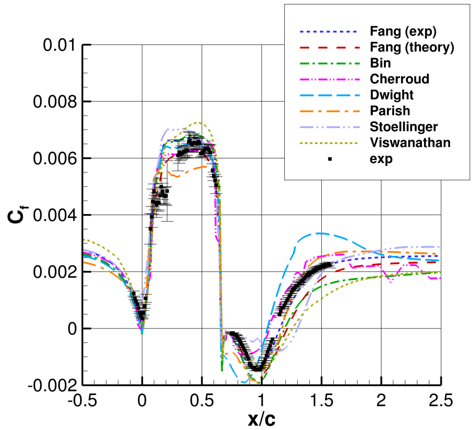


(b) Profiles of u velocity at $x/D_{jet} = 5$

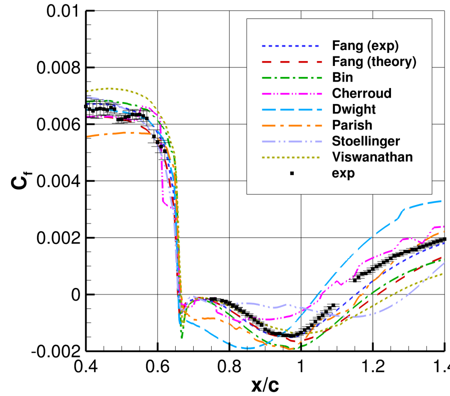


(c) Profiles of $\langle u'v' \rangle$ at $x/D_{jet} = 5$

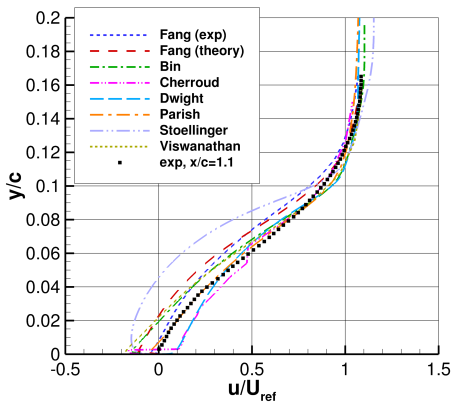
Figure 2. ASJ case: axisymmetric jet.



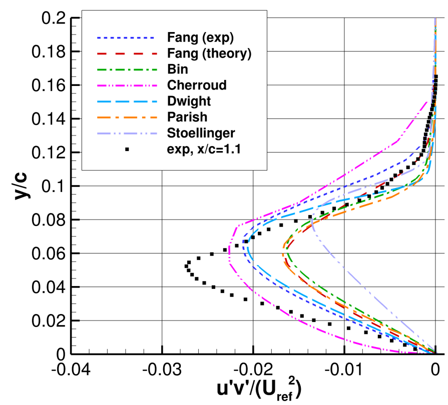
(a) Skin friction coefficient



(b) Skin friction coefficient (zoom)



(c) Profiles of u velocity at $x/c = 1.10$



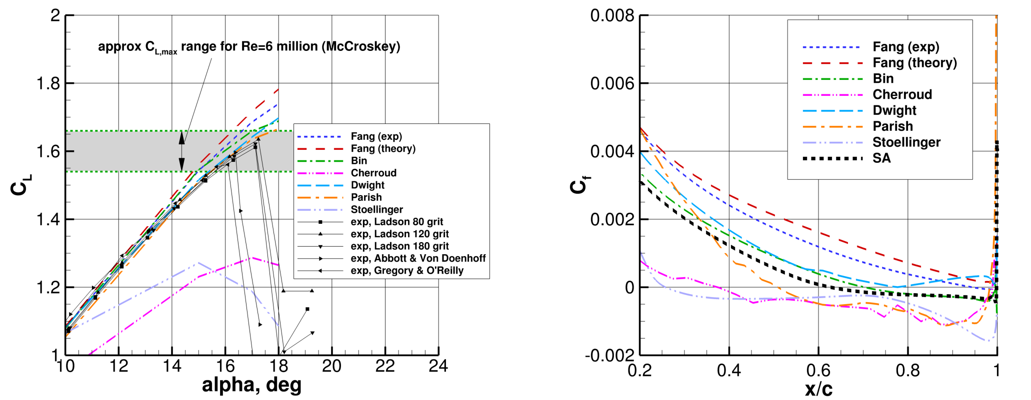
(d) Profiles of $\langle u'v' \rangle$ at $x/c = 1.10$

Figure 3. 2DWMH case: NASA wall-mounted hump.

$5 < x/D_{jet} < 10$. Figures 2(b) and (c) show u velocity and turbulent shear stress profiles at $x/D_{jet} = 5$. Some nonphysical kinks/nonsmoothness appears in a few of the solutions.

For 2DWMH, there were significant deviations between the participant results, as shown in Figs. 3(a) and (b). For this case, standard RANS models tend to predict flow reattachment too far downstream (often near $1.2 < x/c < 1.3$), rather than the experiment's $x/c \approx 1.1$. Five of the participant results yielded reattachment upstream of $x/c = 1.2$, in better agreement with experiment than typical RANS models. However, in two cases, reattachment occurred too early, well upstream of the experimental data. The large variation in participant results was even noted far upstream, prior to flow separation, and even in the flat plate flow leading up to the start of the hump. Examples of velocity and turbulent shear stress profiles are shown in Figs. 3(c) and (d) at $x/c = 1.10$, near the location where the flow reattached in the experiment. Here, again, large differences in the participant results are evident. None agreed particularly well with the measured turbulent shear stress profile, but one or two showed reasonably close agreement with parts of the measured velocity profile.

Finally, for 2DN00, lift curve results are shown in Fig. 4(a) and upper surface skin friction results are shown for the highest angle of attack of $\alpha = 18°$ in Fig. 4(b). Five of the participants produced reasonable lift curve behavior, in line with the experimental data (although tending to overpredict the lift near $C_{L,max}$). For upper surface skin friction coefficient at $\alpha = 18°$, no experimental data



(a) Lift curve (b) Upper surface skin friction coefficient at $\alpha = 18°$

Figure 4. 2DN00 case: NACA 0012 airfoil.

exists, but standard SA results (thick black dashed line) are included for comparison. While SA indicated a separation location of about $x/c = 0.62$, the participant results gave a very large range from $x/c = 0.26$ to fully attached.

The Collaborative Testing Challenge proved to be a difficult challenge for most of the participants. It was hard to perform well for all test cases. Although (on the plus side) the participants were each able to use a single strategy to yield plausible results for the diverse cases, there was (on the minus side) a broad range of very different solutions. Also, in some cases, results included curves that were nonsmooth. Sometimes, those who performed best for one or more of the cases produced worse results for others. And models that agreed well with one another for one case often produced very different results in another case. In the end, the symposium participants appreciated the value of this exercise, especially because seeing a variety of models and methods applied to the same problems (and plotted together) helps shed light on the state of the art. There is an interest in seeing these types of challenge cases carried forward to future events.

6 Summary, recommendations, and future directions

In summary, from the symposium, it is clear that there exists a dedicated community of interested researchers in the area of data-driven turbulence and transition modeling (DDTTM). These researchers include turbulence modelers, ML experts, and CFD coders and practitioners. This symposium and other meetings like it are good ways to bring the experts together, to forge professional working relationships and connections, and to help accelerate further progress in this area. It was noted that in DDTTM we are currently very far from having a common language. Perhaps through continued interactions, the culture can be better aligned.

At this point in time, we are seeing isolated successes of machine learning applied to turbulence modeling in the literature, but these successes tend to have a very narrow focus, with applicability primarily to narrow ranges of problems. At this symposium, it was made clear that the RANS application community has not yet gotten anything usable or useful from ML work to date. In particular, the RANS application community needs fully published models that are universal, in the sense that they can be used by anyone and applied to as many flows as possible without concern for unusual or detrimental behavior. To be clear, ‘universal’ in this context does not mean that they can predict every type of flowfield well, but rather that it makes improvements in at least some key areas (such as for separated flows), while doing no harm in others. There are also many constraints and best practices associated with RANS turbulence model development that are sometimes violated by ML practitioners, either out of expediency or lack of knowledge. However, this field is still emerging. It is hoped that by continuing to actively communicate needs and capabilities between the disciplines, the constraints and best practices will be better followed, and useful advances will emerge.

Some specific recommendations emerged from this symposium. Like the 2017 symposium, many of them center around continuing to hold specialists meetings like this.

- Keep the symposium series going, possibly every 2 or 3 years. In addition to the University of Michigan and NASA, try to have different organizations serve as sponsors.
- NASA alone cannot sustain coordination efforts; instead, a committee or small team of leaders from different interested organizations is needed to meet regularly, make decisions, and organize events.
- Hold other meetings, workshops, or special sessions in conjunction with larger conferences, such as AIAA, ETMM, ERCOFTAC, etc.
- Continue the collaborative challenge, aligned with future meetings and/or via an online call for input and virtual evaluations.
- Create an online documentation website hosting this group's activities. This site could be used to list the most useful papers on the subject of DDTTM, provide templates on how to document methods and maintain common/consistent nomenclature, provide or point to useful high-fidelity datasets, post new models, and/or archive comments and conversations.
- Start to share codes/models/architectures for better openness and reproducibility.

Moving forward, a small, informal group has already been established to look into initiating a few actions and events in the near future. These include establishing a Special Interest Group (SIG) within ERCOFTAC, holding a mini-symposium at ETMM14, and working toward a possible stand-alone symposium in Europe in 2024. Other events are possible, including special sessions at future AIAA conferences.

Based on the overall discussions from the symposium, the field of ML has a long way to go before general improvements to turbulence models may be seen. In other words, the payoff (if any) will probably not be immediate. However, ML-related activity worldwide is clearly increasing, and some progress is being made in specific turbulence modeling applications. As the field matures, researchers will eventually adopt a common language, rules and best practices will be more broadly shared, and goals will become more universal and well understood. Therefore, we feel that it is important to remain engaged at some level of (research) effort, to stay abreast of developments in the literature as well as to contribute to coordinated activities in the field.

As more researchers learn to use widely available ML tools, and attempt to apply them toward the improvement of turbulence or transition models, it is hoped that the existing DDTTM community can help provide valuable guidance and offer useful forums, with better data-driven models emerging as a result.

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APPENDIX - List of talks and panels from the 2022 Symposium on Turbulence Modeling: Roadblocks, and the Potential for Machine Learning

- Keynote: An Old-Fashioned Framework for Machine Learning in Turbulence Modeling (Philippe Spalart, Retired, NASA/Boeing)
- Reynolds-averaged Navier-Stokes (RANS) related talks
  - A data-driven wall law for the mean velocity in adverse-pressure gradient and modification of the SSG/LRR-w model (Tobias Knopp, DLR)
  - Improvement on the AMM model for predicting wing-body juncture flows (Hiroyuki Abe, JAXA)
  - Review & Potential of Wray-Agarwal Family of Turbulence & Transition Models for RANS Simulations (Ramesh Agarwal, Washington University)
  - Measurement and Modeling of Non-Equilibrium Turbulent Boundary Layer Flows (Danny Fritsch, Virginia Tech)
  - Benchmark Turbulence Modeling Validation Experiments for Three-Dimensional Flows with Separation (Todd Lowe, Virginia Tech)
- Invited Talk: The Anchor Points of Turbulence Modeling (George Huang, Wright State University)
- Panel: Reynolds-averaged Navier-Stokes (RANS) (Paul Batten, Metacomp Technologies; Paul Durbin, Iowa State University; Charles Hirsch, Cadence-Belgium; Brian Smith, Lockheed-Martin), Moderated by Philippe Spalart, Retired, NASA/Boeing
- Talks including the Collaborative Testing Challenge
  - Introduction to the Collaborative Testing Challenge (Chris Rumsey, NASA Langley)
  - V&V of DES using multiple CFD codes; and Collaborative Testing Challenge (Michael Stoellinger, University of Wyoming)
  - Spatial Model Aggregation (X-MA) of stochastic Explicit Algebraic Reynolds Stress models (Soufiane Cherroud, Arts et Metiers Sciences & Technologies)
  - Towards more accurate and general turbulence models using CFD-driven training on multiple flows (Yuan Fang, University of Melbourne)
  - A data-driven turbulence modeling framework for the Reynolds-averaged Navier-Stokes equations via discrepancy-based tensor-basis neural networks (Eric Parish, Sandia National Laboratories)
  - Progressive, Extrapolative Machine Learning for Turbulence Modeling (Jaiqi Li, Pennsylvania State University)
  - Turbulence Closure Modeling with Differentiable Physics (Venkat Viswanathan, Carnegie Mellon University)
  - Field Inversion and Machine Learning Approach for Improved Turbulent Predictions of Flows over Airfoils (Koushik Marepally, University of Maryland)
  - Challenge entry: SpaRTA with classification (Richard Dwight, TU Delft)
- Invited Talk: Recent evolution of Gene-Expression Programming for developing turbulence models (Richard Sandberg, University of Melbourne)

- Invited Talk: The HiFi-TURB EU project: Vision and Progress of ML-based Turbulence Modeling (Charles Hirsch, Cadence-Belgium)
- Machine Learning (ML) related talks
  - Developing hierarchical augmentations via the "Learning and Inference assisted by Feature-space Engineering (LIFE)" framework (Vishal Srivastava, University of Michigan)
  - Using LES/DNS Data for Neural Network-based Improvement of Existing Turbulence Models (Paul Orkwis, University of Cincinnati)
  - Toward the use of convolutional neural networks as a post-processing enhancement to RANS-modeled turbulence (John Romano, Naval Surface Warfare Center)
  - Potential of Data Driven Methods for Reynolds Stress Modeling-A Fundamental View (Bernhard Eisfeld, DLR)
  - Machine Learning, Scale Resolving Simulations and the Future of Predictive Computations of Engineering Flows: A perspective (Sharath Girimaji, Texas A&M)
  - Data-Driven Calibration of RANS Closure Models with PIV (Nathan Miller, Sandia National Laboratories)
  - Data-Driven Construction of Iterative Algebraic Reynolds Stress Models using Model-Derived Turbulence Variables (John Evans, University of Colorado Boulder)
  - Lessons from Data-driven Reynolds Stress and Turbulent Scalar Flux Closures (Andrew Banko, US Military Academy West Point)
  - Improvement of RANS models by machine learning for a bump configuration (Pedro Volpiani, ONERA)
- Panel: Machine Learning (ML) (Andrew Banko, US Military Academy West Point; Paola Cinnella, Sorbonne University; Richard Dwight, TU Deflt; Sharath Girimaji, Texas A&M; Robert Moser, University of Texas Austin), Moderated by Karthik Duraisamy, University of Michigan
- Keynote: Conjectures of a Generalized Law of the Wall and a Structural Limitation for Classical Turbulence Models (Philippe Spalart, Retired, NASA/Boeing)
- Transition related talks
  - Current status of PDE-based transition modeling for aerodynamic applications (Jim Coder, Penn State University)
  - Hybrid closure modeling with laminar to turbulent transition (Paul Durbin, Iowa State University)
  - High-Fidelity Computational Data of Transitional Boundary Layers for a Data-Driven Approach (Solkeun Jee, Gwangju Institute of Science and Technology)
- Panel: Transition (Karthik Duraisamy, University of Michigan; Heng Xiao, Virginia Tech), Moderated by Paul Durbin, Iowa State University

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14. ABSTRACT
A three-day symposium sponsored by NASA was held in July 2022 in Suffolk, Virginia on the subject of Turbulence Modeling: Roadblocks, and the Potential for Machine Learning. This meeting brought together over 80 experts from academia, government, and industry to discuss critical issues for Reynolds-averaged Navier-Stokes turbulence and transition models, as well as to evaluate the results from a collaborative testing challenge based on data-driven methods and machine learning technology. This report puts this symposium in context with an earlier similar meeting and summarizes many of the questions, discussions, and conclusions that arose from it. Next steps are suggested.

15. SUBJECT TERMS
turbulence modeling, machine learning

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