



The Pivotal Roles of Model Validation Maturity in Advancing the Capabilities and Adoption of CFD

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ABSTRACT

Subtle differences in the way in which CFD validation is perceived can have profound implications for the ways in which CFD capabilities are developed and deployed. By appealing to systems engineering principles, the evolutionary nature of model validation objectives throughout the development lifecycle is outlined. The concept of CFD validation maturity is introduced to place these observations in context. CFD model development lifecycles are shown to be extended and federated across multiple stakeholders. This broad situational awareness allows the mutual dependencies between the developer and user communities to be re-interpreted in a manner that is consistent with the use of model validation metrics. The potential utility of such metrics in simultaneously monitoring and guiding the maturation of a CFD model's development and use is outlined. Finally, in view of the acknowledged limitations of current set-based approaches to CFD validation and given the time that has elapsed since community-based guidance on CFD validation was last updated, it is recommended that the existing guidance be revised to reflect contemporary understanding and experience.

1.0 INTRODUCTION

Ideally, industrial users of a computational model would like to know how accurate the outputs produced by the model are considered to be (and for this information to be evidence-based), not how accurate they *ought* to be (requirement-based). Moreover, they would like to know this information for a suitably wide range of model inputs *before* the model is used, so that the expected accuracy of the model may be compared with the accuracy requirements for the task at hand.

Despite the apparent simplicity of the rationale underlying the above assertions, the practical realization of this situation with regards to Computational Fluid Dynamics (CFD) poses a number of challenges. The scope of the most recently issued ASME Standard for verification and validation in CFD[1] provides a perspective on one of them:

"The objective of this Standard is the specification of a ... validation approach that quantifies the degree of accuracy inferred from the comparison of [computed] solution and [measured physical] data for a specified variable at a specified validation point. ... Consideration of the accuracy of simulation results at points within a domain other than the validation points (e.g., interpolation/extrapolation in a domain of validation) is a matter of engineering judgment specific to each family of problems and is beyond the scope of this Standard."

Industrial concerns about focusing CFD validation approaches on single "validation points" have been expressed for many years (see e.g. [2]). In the spirit of this workshop, this paper illustrates how a broader appreciation of the ways in which CFD validation is viewed may have profound implications for the ways in which CFD capabilities are both developed and used. The principal dimension considered is CFD model validation maturity.



In Section 2, CFD model validation is reconsidered in the light of the principles of systems engineering. On the basis of the attendant observations, Section 3 provides an overview of some of the challenges and opportunities facing the developer and user communities. Finally, a succinct set of closing remarks and recommendations are provided in Section 4.

2.0 CFD MODEL VALIDATION MATURITY

2.1 Wider Context

Widespread use of the term "validation" in engineering contexts appears to have been stimulated by the development of formal techniques to control the development of computer software that emerged in the latter half of the twentieth century. The origins of the Systems Engineering "V" – and with it, its definition of validation – have been traced in this way.[3] In systems and software engineering, validation is considered a generic process with a specific purpose, defined[4] as follows:

"The confirmation, through the provision of objective evidence, that the requirements for a specific intended use or application have been fulfilled."

It is important to recognize that a validation process should be applied at various stages throughout the development lifecycle and that, in each case, it is bounded by inputs and outputs appropriate to the lifecycle stage. These define, by mutual agreement with the relevant stakeholders, what it means for something to be "validated" (with whatever caveats are appropriate) at a given stage in the lifecycle. Thus, in [4], the description of validation as "the set of activities that ensure and provide confidence that a system is able to accomplish its intended use, goals, and objectives (i.e., meet stakeholder requirements) in the intended operational environment" is refined, progressively, through the lifecycle to "evaluation of the capability of the delivered system to meet the customer's operational need in the most realistic environment achievable".

In the context of the routine industrial use of a CFD model, a realistic operational environment would be one in which, on any given day, it might be called upon to support the characterization of various aspects of the aerodynamic performance of multiple airframes, each of which may be at a different stage in its development. Generally speaking, a particular CFD model will be only one of several simulation options that may be brought to bear in any given scenario. In these circumstances, the scope and potential diversity of applications and approach provide both challenges and, as will be explained in Section 3, opportunities for CFD model validation.

Apparently sharing similar heritage to that outlined above, the concept of CFD validation emerged towards the end of the 1980's.[5] The wording of the definition originally adopted by the AIAA in 1998[6]:

"The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model"

remains unchanged and is now used by a number of bodies, including ASME[1]. On the face of it, the AIAA definition[6] appears broadly consistent with the more generic ISO definition[4] cited above. However, the extant CFD validation literature has relatively little to say on the subject of how the requirements imposed on a model validation activity may be expected to change as the model progresses through its development lifecycle. There are many possibilities here. However, for the purposes of this paper, we focus on only two broad types of scenario:

- Those in which the state of the model is considered to be subject to ongoing change or refinement. For the reasons set out in Section 2.3, this will be referred to as a model developer perspective.
- Those in which the model design is essentially considered to be fixed. For the reasons set out in



Section 2.3, this will be referred to as a model user perspective.

2.2 Model Validation Assessment

When validating aerodynamic models in MBDA, it is customary to make clear the distinction between model accuracy quantification (comparison of model outputs with physical measurements) and model validation assessment (comparison of the model accuracy with validation metrics) and to assert that <u>both</u> are fundamental components of model validation. The manner in which this is accomplished is illustrated in Figure 1. For CFD model validation, this differs from the logic expressed in [1] (which is represented in Figure 2) in several important regards. In the context of the current paper, the most important differences are associated with the nature of the validation metrics (Figure 1) and validation requirements (Figure 2) employed.* In Figure 2, these are based on external criteria (requirements) imposed on the modelling activity and are usually considered to be fixed. However, in Figure 1, in addition to reflecting the demonstrated status of quantified model accuracy, they act as repositories for the types of engineering judgement cited in Section 1[1]. Consequently, they are updated regularly to account for the accumulation of experience and insight into the behavior of the model being validated. Thus validation metrics serve as both a proving ground and the source of stimulus for progressive refinements to their formulation. A typical pattern of use is outlined below.

As experience in validating a model is accumulated, the metrics employed become increasingly informed by demonstrated model behaviors. Provided no "surprises" are encountered (these will require further investigation and, potentially, either re-formulation of the model and/or the metrics), the metrics will follow convergent paths during the course of successive validation assessments. Consequently, a point will be reached where the range of input conditions covered will have provided sufficient opportunity to confirm the predictive capability of the engineering judgement encapsulated in the validation metrics. This constitutes a quantitative basis for process closure. Once established, the predictive capability may be subject to subsequent refinement, by expanding its perimeter and/or refining the confidence associated with it.

The course taken in pursuit of process closure is followed empirically, guided by the observations accumulated during successive validation assessments. According to Figures 1 and 2, the first factor influencing the course of subsequent events is the extent of compliance demonstrated with the validation criteria being used. Initially, we consider the circumstances that may arise if model accuracy quantification is deemed non-compliant; scenarios in which the outcome is deemed to be compliant will be addressed in Section 3, below.

In the case of a non-compliant outcome, the options essentially fall into two broad categories, distinguished by a decision to either re-formulate the model or re-formulate the validation criteria in some way.[†] The outcome will be determined by who is making the decision and, more importantly, where the stakeholders consider they are in the model development lifecycle (as per Section 2.1, above).

^{*} Differences associated with the concept of a validation hierarchy and the description of physical referent data as being "experimental" are addressed, succinctly, in Sections 3.3 and 3.4, respectively.

[†] This decision may be postponed, either (i) temporarily, by continuing without re-formulating either, in the hope that the additional information gained in subsequent validation activities (undertaken with different model inputs) will help decide on the best course of action to take, or (ii) more permanently, if no value in continuing validating the model is identified.



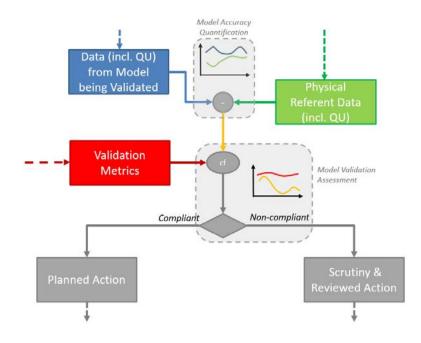


Figure 1: Schematic Stencil of a Single Model Validation Activity Post Preparation of Model & Referent Data and Updating of Validation Metrics (NB: QU = Quantified Uncertainty; cf = compare with)

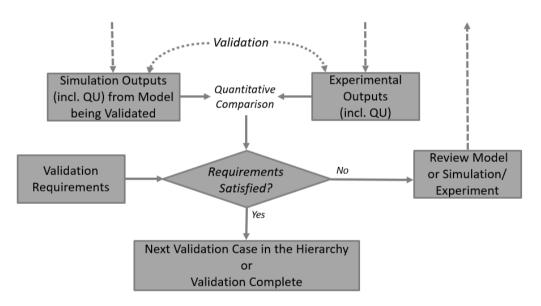


Figure 2: CFD Model Validation Logic Post Preparation of Model & Referent Data according to [1] (NB: QU = Quantified Uncertainty)

2.3 Perspectives on CFD Model Development Lifecycles

The general patterns of development followed by CFD models and flight vehicles differ in several important respects. In the context of the current paper, one of the most important distinctions is the nature of the validation processes completed prior to making them available to their intended users. There are many reasons why the processes adopted differ, and why certification and acceptance of CFD models is not regulated by independent statutory bodies (the reduced immediacy of the potential risk to human life, for



instance). Beyond noting that these differences exist, further analysis of this subject is beyond the scope of this paper. However, these differences in lifecycle do have profound consequences for CFD model validation, in particular its maturation and the increased responsibilities placed on the user community to facilitate it.

Returning to the question as to whether to re-formulate the model or the validation criteria: From the perspective of an industrial aerodynamicist, the former option may either (i) not be available (if one does not have immediate access to a practicing model architect or the means to implement a re-formulated model into an accessible CFD workflow), or (ii) not be available in a suitable timescale.* In these circumstances, the only option available is to re-formulate the validation criteria, by reducing either the stringency or scope of the accuracy metrics, or both.

At first sight, moving the goalposts in this way this might seem to be contravening a basic tenet of validation, essentially reducing the purpose of model accuracy quantification to one of characterization. While there may be an element of truth to this, there are a number of potentially mitigating factors. These include: (i) the assertions made at the beginning of this paper concerning the fundamental user requirement to be able to apply a model, in a predictive capacity, over a wide range of input conditions; (ii) it is not reasonable to expect that all potential uses of a model will be known at the point of its formulation (or, more precisely, the point at which accuracy requirements were initially imposed on it for a given application); (iii) model accuracy requirements may be subject to change over time anyway.[†] It should also be recognized that the primary purpose of validating a model of a missile's aerodynamic characteristics via flight testing is to confirm that the aerodynamic behavior derived from in-flight measurements is consistent with that predicted by the model (i.e. the reason for conducting this type of validation assessment is not to obtain a direct comparison with externally imposed requirements).

Given the diversity of aerodynamic characterization activity that may be ongoing at any one time in an industrial setting, there is usually a spectrum of potential utility rather than a single application for any given modelling capability. Thus, from a model user perspective, the ultimate intent of CFD model validation is usually to characterize the behavior of the model so that it may be used in a predictive capacity, such that judicious choices may be made concerning its use alongside the other available modelling and simulation techniques. The availability of multiple CFD models compounds this task somewhat.

Even in circumstances where model re-formulation is an active proposition, the accuracy requirements being imposed are not usually considered absolute criteria for success or failure. Indeed, given the complexity of the aerodynamic behaviors being simulated, it is often enough for discernable improvements over prior computed results to be observed for a new or updated model to be made available to the user community (in the hope that this will facilitate wider validation and, hence, progress). To illustrate this point, one of the most widely used turbulence models in the aerospace community (that attributed to Spalart and Allmaras[7]) has been subject to several "mid-life updates" over the course of the past 25 years, with the most recent dating from 2020.[8] Thus, while the development lifecycles for particular CFD models may appear to be

^{*} Note the decision to re-formulate a model is distinct from selecting an alternative model to validate.

[†] In the author's experience, there are several reasons why this may be the case. For instance, the external requirements imposed on a missile system rarely (if ever) include specific requirements for aerodynamic data accuracy. Thus, aerodynamic data accuracy requirements are derived via a systems-based decomposition of the overarching functional requirements; they are therefore subject, to a greater or lesser extent, to negotiation during the course of developing a balanced design of the system as a whole. Furthermore, in many cases, the levels of accuracy sought during the earliest stages of the lifecycle are less stringent than those employed during the later stages.



dormant from afar, this is not necessarily the case: model development may still be active, albeit over an extended and federated lifecycle.*

The following section identifies some of the challenges faced in establishing CFD model validation maturity. In line with the objectives of this workshop, opportunities for building – or reinforcing – bridges between model developers and industrial model users are also highlighted. The material is derived from the recent experience of the author and is meant to stimulate discussion at the workshop rather than be considered comprehensive or definitive. In view of the importance of what the ASME standard[1] refers to as engineering judgement between validation (set) points, the material is presented under the heading of "Situational Awareness".

3.0 SITUATIONAL AWARENESS

A key consideration to address in developing a predictive CFD capability is the nature of the reliance on physical referent data, especially in situations where it is not practically possible to secure it. In this paper, focus is placed on "interpolative" scenarios, i.e. those in which physical referent data could be sought, if required. Brief indication is provided as to how these insights might be extended to permit modest extrapolation. However, the maturation of CFD model validation in circumstances well beyond those for which physical referent data may readily be acquired is beyond the scope of this paper.[†] Throughout, the intent is to illustrate the pivotal roles that CFD model validation maturity can play in determining the directions in which CFD development and use are pursued. These will be addressed from four perspectives: distinguishing between cause and effect, establishing validation dialog, the importance of computational experimentation, and the reliance on physical referent data.

3.1 Distinguishing between Cause and Effect

[10], a document published to help interpret the ASME standard[1], makes it clear that the conclusiveness of model accuracy quantification is dependent upon the uncertainty in the referent physical data and the accuracies of both (i) the numerical simulation and (ii) the definition of the model input parameters. Thus, a wide range of factors can have a profound impact on CFD model validation. Recent experience in the Missile Facet of a NATO STO Task Group, AVT-316 [11-22], has highlighted both the potential magnitude of the contribution that may be made by numerical error in this regard and the difficulties that may be encountered in its estimation, even for the simplest of vortex dominated flows.

To illustrate, Figure 3 presents rolling moment coefficient data computed for a generic cruciform missile airframe over a range of aerodynamic roll angles, demonstrating its sensitivity to the resolution of the flow afforded by the computational mesh (all other factors remaining constant). The sensitivity observed is most pronounced over a limited range of roll angles and for the coarsest levels of mesh resolution. This variation in sensitivity has been attributed primarily to (i) numerical dissipation in the computations (which can be pronounced in the vicinity of vortices), and (ii) the proximity of the passage of vortices past the tail control fins, rather than any fundamental behavioral differences in the aerodynamic phenomena being modelled.

^{*} In the context of this workshop, it is interesting to note that the extent to which CFD model architects of [8] have been influenced by the results and observations of others may be considered evidence of the bridges that currently exist between model developers and model users.

[†] It is interesting to note that effort is underway[9] to redress both the interpolative and extrapolative shortfalls in the scope of the current ASME standard.[1] The author was unaware of the directions being pursued in these regards in preparing the material presented herein.



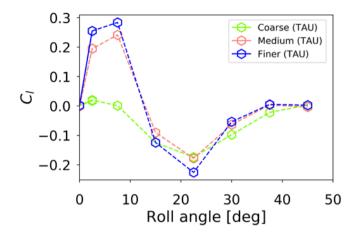


Figure 3: Sensitivity of computed total rolling moment coefficient to mesh resolution as a function of aerodynamic roll angle for the OTC1 airframe (from [11])

The point being made here is that it is important to distinguish between cause and effect: the relationship between any form computational error (whatever its source – numerical or modelling) and its integrated effects on the overall aerodynamic characteristics of an airframe may be highly non-linear. This clearly has important potential implications for establishing a predictive capability and may require additional, more localized, flow behavioral metrics to be used to guide CFD model validation assessments.

A corollary to this observation is that if one is seeking to validate a CFD model, it is better to include flow conditions which exhibit clear metrics in the model validation process: had the AVT-316 activity associated with Figure 3 been focused at roll angles closer to 45° (at the expense of those closer to 0°), a different set of conclusions may have been drawn. As will become apparent, both the developer and industrial stakeholder communities may play important – and mutually beneficial – roles in identifying suitable behavioral characteristics to include in CFD model validation metrics and selecting conditions for which physical referent data should be sought to facilitate CFD model accuracy assessment.

3.2 Establishing Validation Dialog

As noted above, a wide range of factors need to be addressed when undertaking a CFD model validation activity. Indeed, a thorough understanding of the underlying principles and practicalities of both the computational and physical testing techniques being employed is essential to the pursuit of CFD model validation. For instance, detailed attention must be paid to all aspects of CFD verification (from code verification through to solution verification) to ensure that the computational models are being solved correctly (i.e., without coding errors) and to a quantified numerical accuracy. Without this, there is increased risk of misinterpreting and incorrectly attributing or quantifying the reasons for, or magnitude of, any residual disparity in the computed and measured data. Figure 3 provides a perspective on the magnitude of the potential difficulties that can be encountered in this regard if solution verification is not addressed. While not apparent in this Figure, the AVT-316 Missile Facet also identified a number of shortfalls in the conventional techniques for quantifying discretization error[13]. Any developments that can be made to improve this situation will therefore have a direct impact on CFD model validation.

Experience[23] has shown that ensuring computational and physical testing activities are undertaken in balanced and synergistic ways throughout can be vital in improving the conclusiveness of the outcomes of validation activities, whether the capability being validated is a physical testing technique or a CFD model. This synergy is referred to as validation dialog since (i) it usually involves the active participation of multiple stakeholders and (ii) it is most effective when informed by the computational and physical testing techniques



"speaking for themselves" – a process by which computational and/or physical data are subjected to detailed, systematic scrutiny. The latter provides a powerful mechanism for identifying features that might otherwise go unnoticed or be misinterpreted. By appealing to the various mutual accountabilities that exist between the computational and physical techniques being employed[24], it also reduces reliance on heuristic judgement. Validation dialog generally serves to accelerate the pace of learning for all participants and enhance the benefit gained from each activity pursued.

In seeking to identify suitable behavioral characteristics to include in CFD model validation metrics, it may be beneficial to establish new (or improved) avenues of validation dialog between model developers and industrial users. From the perspective of an industrial aerodynamicist, any insights that could be afforded concerning the reasoning that led to the original formulation – or subsequent revisions – of the model being validated, including any anticipated constraints or limitations, would be extremely valuable. Moreover, recalling the intent to establish an active validation dialog, it would be particularly helpful if such insights were supported by illustrated, physical reasoning – including comparative traits with similar models – where possible. The synergistic benefits will likely be felt most immediately in the quality of the feedback provided by users, whose observations drawn from their experience of using the model would be better informed and, therefore, more incisive. An active validation dialog will also help model validation metrics to be maintained and kept up-to-date with the outcomes of relevant model validation assessments.

3.3 Computational Experimentation

The potential utility of computational experimentation in the pursuit of CFD model validation maturity should not be underestimated.^{*†} Of the various potential uses that have been identified or proven to date (see [22] and [23] for some examples), we focus on only one here: namely the potential utility of multi-fidelity simulations. These may be used to help identify (i) the CFD model behavioral traits being sought to augment model validation metrics and (ii) the nature and scope of the physical data required to populate such metrics. The essential idea here is to identify distinctive model behavioral traits by assessing the sensitivity of computed flows to the extent of their dependence on the model being validated.

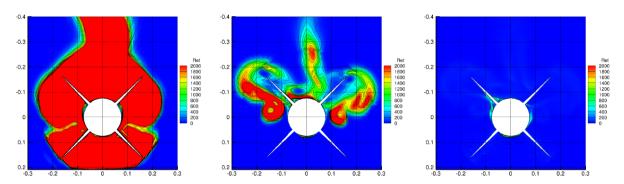
The use of hybrid RANS modelling techniques is well-suited to this, since reliance on the turbulence model (the most common target of CFD model validation) used throughout the flowfield in most Reynolds-Averaged Navier-Stokes computations, is invoked only at sub-grid scale for large regions of the flow when using Delayed Detached Eddy Simulation techniques, for instance. To illustrate, Figure 4 presents some more results produced by the AVT-316 Missile Facet: the reduced magnitudes of eddy viscosity, accompanying reduced dependence on the Boussinesq hypothesis (i.e. moving from left to right in the Figure), are apparent together with the attendant impact on the local distributions of total pressure.[‡]

^{*} In the author's opinion, the terminology adopted in [1] is unfortunate. By appearing to consider experimentation synonymously with physical testing, not only does it convey a misleading impression regarding the manner in which physical tests may be conducted (strict adherence to stringent process is standard practice in industrial wind tunnels, for example) it also fails to draw attention to the potential utility of computational experimentation.

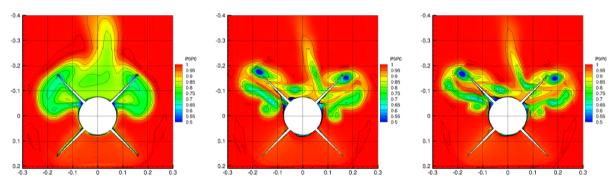
[†] In addition to the potential utility of computational experimentation, even subtle changes to the way in which CFD models are exercised can have profound effects on the ways in which the computations are approached and results received. These can have important implications in the context of developing a predictive CFD capability. The benefits of undertaking computations "blind" (i.e. without sight of physical referent data), as outlined in [22] and [23], provide simple examples of this.

[‡] The examples presented in Figure 4 are based on comparing data predicted using RANS as a baseline, reflecting the fidelity of governing equations currently in routine industrial use. Similar approaches could be adopted with higher fidelity baselines, at higher spatial and temporal resolutions, to inform decisions concerning physical data measurement requirements at very small scales. Note that such decisions will also involve tailoring the requirements to the available metrological techniques and technologies.





a) (Time-averaged) Ratios of eddy to molecular viscosity



b) (Time averaged) Total pressure ratios

The value of the insights that may be gathered in this way is still to be established in practice. However, with the increasing use of hybrid-RANS techniques and the potential use of emerging technologies like geometric deep learning to identify patterns not discernable by human eye, the prospects are surely improving. After all, it stands to reason that it should be easier to study the behavioral traits of a CFD model in a digital environment than in a physical one.

3.4 Reliance on Physical Referent Data

As noted in Section 3.0, above, one of the principal challenges facing the establishment of a predictive CFD capability is that this must be accomplished using limited physical referent data. With the introduction of model validation metrics, this challenge may be re-expressed as determining how to mature the metrics to the point at which they define both the accuracy and scope of input conditions for which the model may be used with confidence (however this is quantified).

The approach endorsed by the ASME Standard[1] is to establish a model validation hierarchy and to progress from one case to the next (see Figure 2). The implementation of this approach has recently been the subject of further scrutiny by another NATO STO Task Group: AVT-297. This Task Group is in the process of producing its final report, so it would not be appropriate to report further on this work herein. Suffice it to say that the author believes that progress is likely to be made more empirically than the manner implied by Figure 2.

To avoid perpetuating the current situation, where CFD model validation guidance is confined to isolated set points,[1], future efforts should gather referent data over focused ranges of conditions. Ideally, these should

Figure 4: An example of multi-fidelity analysis – comparison of data in the fin mid-chord plane for the OTC1 mandatory test case for three modelling scenarios (From left to right: kw-SST (RANS), kw-EARSM (RANS), kw-SST (SAS); from [18])



be selected to straddle conditions which yield a distinct change in flow behavior (the onset of boundary layer separation or collapse of leading edge suction, for instance). This will aid detection (and comparison) of key behavioral traits in the measured and computed flows and, consequently, help formulation of candidate criteria to include in model validation maturity metrics.

Insights acquired via extant physical data are likely to play an important role here (even if the data were not originally acquired for the purpose of supporting CFD validation). For instance, localized changes in airframe stability characteristics with changes in incidence (pitch, roll or yaw) point to significant events occurring in the flow development. If these are either not recovered or are reproduced differently in CFD computations, such circumstances could make good candidates for further study^{*} – or points of entry into model validation experiments[23] – especially if they occur in important regions of the operating envelope. Further pragmatism and economy may be realized (in the form of clearly bounded statements regarding the scope of physical data measurement requirements, for instance) as a result of pursuing carefully focused computational experimentation. While the irony of relying on such computations to guide the physical testing should not be lost,[23] their subsequent connection with physical data may provide a valuable augmentation to the snapshot being formed of the current status of the predictive CFD capability.

As explained in Section 2.1, immediate priorities for physical referent data will likely be influenced by perceptions regarding (i) the development status of the CFD model being validated and (ii) the nature of the requirements imposed on the validation activity. While differences in priority may exist between model developers and industrial users, the simplified analysis reported above has identified potential common ground in the form of CFD model validation metrics, together with a number of mechanisms for building upon it. Whether these metrics are used to improve the ability to anticipate and characterize deficiencies in computed fluid behavior, or to provide stimulus for the formulation of improved models, the potential of their progressive maturation offers benefits to all stakeholders at all stages of CFD model development.

4.0 CLOSING REMARKS

By examining the development lifecycle of a CFD model in the light of systems engineering principles, this paper has identified a range of perceptions regarding what CFD model validation actually means in practice. For those actively involved in model development, their validation objectives are likely to be focused around devising or refining models, potentially to address externally imposed targets. Meanwhile, those primarily engaged in using models that are delivered to them will likely be more immediately concerned with the *a priori* characterization of their behaviors.

Recognition of the extended and federated nature of a CFD model development lifecycle has also allowed the mutual dependencies between the developer and user communities to be re-interpreted. This broader situational awareness is consistent with the use of model validation metrics and their potential utility in simultaneously monitoring and guiding the maturation of a CFD model's development and use.

In view of the time that has elapsed since community-based guidance on CFD validation was last updated, it is recommended that the existing guidance be revised to reflect contemporary experience and understanding. For instance, there is considerable overlap between model credibility and model validation maturity (see e.g. [25,26]). Recognizing that the views expressed herein are those of only one stakeholder, it is hoped that this workshop will provide the stimulus for concerted action in this regard. Given the wider importance of computational model validation, the author hopes that the NATO STO community will play an active role in whatever course of action is taken.

^{*} This was the case for the test case based on the DLR LK6E2 airframe being studied by the AVT-36 Missile Facet.[12,20,21] It was also an aspiration that guided the early stages of the NASA Juncture Flow program.[23]



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