ASME VVUQ 1-2022

Verification, Validation, and Uncertainty Quantification Terminology in Computational Modeling and Simulation

AN INTERNATIONAL STANDARD

The American Society of Mechanical Engineers

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FOREWORD

Starting in the 1960s, computer simulations began to dominate engineering analysis for all but the simplest problems. As reliance on these simulations increased, so did the need for systematic processes that could assess whether simulations can be trusted for their intended purpose (i.e., determine if simulations are credible). Many technical communities developed verification, validation, and uncertainty quantification (VVUQ) processes for that purpose. However, these early VVUQ processes tended to be organization- or industry-specific techniques rather than broad-based tools that could be used across the modeling and simulation communities.

In the mid-1990s, practitioners began publishing documents that were focused on VVUQ techniques in general rather than on the specific technical fields or industries using those techniques. In 2001, the American Society of Mechanical Engineers (ASME) formed the Performance Test Code (PTC) 60 Committee to develop guidelines for VVUQ in computational solid mechanics. In 2004, a companion committee, designated PTC 61, was formed to address computational fluid dynamics and heat transfer.

In 2008, an overarching committee, the Verification and Validation (V&V) in Computational Modeling and Simulation Committee, was established to coordinate the efforts across multiple application areas. The PTC 60 and PTC 61 Committees were redesignated as the V&V 10 and V&V 20 Subcommittees, respectively. From 2010 to 2019, five additional ASME V&V Subcommittees were developed. In 2021, ASME renamed the V&V Standards Committee the VVUQ Standards Committee in recognition of the major role of uncertainty quantification in determining the credibility of a simulation. The ASME V&V Subcommittees have likewise been redesignated, as shown in the list below. Each existing ASME V&V standard will be redesignated as an ASME VVUQ standard in its next edition.

Year Formed	Subcommittee
2001	VVUQ 10 Subcommittee — Computational Solid Mechanics
2004	VVUQ 20 Subcommittee — Computational Fluid Dynamics and Heat Transfer
2010	VVUQ 30 Subcommittee — Computational Simulation of Nuclear System Thermal Fluids Behavior
2011	VVUQ 40 Subcommittee — Computational Modeling of Medical Devices
2016	VVUQ 50 Subcommittee — Computational Modeling for Advanced Manufacturing
2017	VVUQ 60 Subcommittee — Computational Modeling for Energy Systems
2019	VVUQ 70 Subcommittee — Machine Learning

The ASME VVUQ subcommittees are in the process of developing standards and supporting publications in each of their respective technical areas. This Standard (ASME VVUQ 1) is intended to provide the ASME VVUQ Subcommittees with a harmonized set of definitions that can be used in all ASME VVUQ standards. This first edition contains selected terms commonly used in the VVUQ processes. Other terms (e.g., model calibration, uncertainty propagation, sensitivity analysis) will be considered in future revisions.

This Standard is available for public review on a continuing basis. This provides an opportunity for additional input from industry, academia, regulatory agencies, and the public-at-large.

ASME VVUQ 1 was approved by the VVUQ Standards Committee on June 30, 2022 and was approved and adopted by the American National Standards Institute on August 8, 2022.

ASME VVUQ COMMITTEE
Verification, Validation, and Uncertainty Quantification in Computational Modeling and Simulation

(The following is the roster of the Committee at the time of approval of this Standard.)

CORRESPONDENCE WITH THE VVUQ COMMITTEE

General. ASME codes and standards are developed and maintained by committees with the intent to represent the consensus of concerned interests. Users of ASME codes and standards may correspond with the committees to propose revisions or cases, report errata, or request interpretations. Correspondence for this Standard should be sent to the staff secretary noted on the committee's web page, accessible at https://go.asme.org/VnVcommittee.

Revisions and Errata. The committee processes revisions to this Standard on a continuous basis to incorporate changes that appear necessary or desirable as demonstrated by the experience gained from the application of the Standard. Approved revisions will be published in the next edition of the Standard.

In addition, the committee may post errata on the committee web page. Errata become effective on the date posted. Users can register on the committee web page to receive e-mail notifications of posted errata.

This Standard is always open for comment, and the committee welcomes proposals for revisions. Such proposals should be as specific as possible, citing the paragraph number(s), the proposed wording, and a detailed description of the reasons for the proposal, including any pertinent background information and supporting documentation.

Cases

(a) The most common applications for cases are

(1) to permit early implementation of a revision based on an urgent need

(2) to provide alternative requirements

(3) to allow users to gain experience with alternative or potential additional requirements prior to incorporation directly into the

(4) to permit the use of a new material or process

(b) Users are cautioned that not all jurisdictions or owners automatically accept cases. Cases are not to be considered as approving, recommending, certifying, or endorsing any proprietary or specific design, or as limiting in any way the freedom of manufacturers, constructors, or owners to choose any method of design or any form of construction that conforms to the Standard.

(c) A proposed case shall be written as a question and reply in the same format as existing cases. The proposal shall also include the following information:

(1) a statement of need and background information

(2) the urgency of the case (e.g., the case concerns a project that is underway or imminent)

(3) the Standard and the paragraph, figure, or table number(s)

(4) the edition(s) of the Standard to which the proposed case applies

(d) A case is effective for use when the public review process has been completed and it is approved by the cognizant supervisory board. Approved cases are posted on the committee web page.

Interpretations. Upon request, the committee will issue an interpretation of any requirement of this Standard. An interpretation can be issued only in response to a request submitted through the online Interpretation Submittal Form at https://go.asme.org/InterpretationRequest. Upon submitting the form, the inquirer will receive an automatic e-mail confirming receipt.

ASME does not act as a consultant for specific engineering problems or for the general application or understanding of the Standard requirements. If, based on the information submitted, it is the opinion of the committee that the inquirer should seek assistance, the request will be returned with the recommendation that such assistance be obtained. Inquirers can track the status of their requests at https://go.asme.org/Interpretations.

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Committee Meetings. The VVUQ Standards Committee regularly holds meetings that are open to the public. Persons wishing to attend any meeting should contact the secretary of the committee. Information on future committee meetings can be found on the committee web page at https://go.asme.org/VnVcommittee.

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VERIFICATION, VALIDATION, AND UNCERTAINTY QUANTIFICATION TERMINOLOGY IN COMPUTATIONAL MODELING AND SIMULATION

1 SCOPE, PURPOSE, AND REFERENCES

1.1 Scope

This Standard provides a harmonized set of definitions for verification, validation, and uncertainty quantification (VVUQ) concepts.

1.2 Purpose

The purpose of this Standard is to give a summary of key definitions and concepts for VVUQ and describe the themes that connect the VVUQ community and ASME VVUQ standards. The intent is to assist the developers and users of computational models to better communicate the evidence that justifies application of their models for the context of use. ASME VVUQ 1 is also intended to provide the VVUQ Subcommittees with terminology that can be used to establish consistency across all VVUQ standards while allowing each subcommittee to adapt the terminology to their own specific requirements.

1.3 References

Paragraph 1.3.1 contains key ASME standards used as references in developing this Standard. Unless otherwise noted, the latest edition of the ASME standards shall apply. In addition, para. 1.3.2 contains other industry publications that were considered while generating the definitions given in this Standard.

1.3.1 ASME Standards

ASME PTC 19.1. Test Uncertainty. The American Society of Mechanical Engineers.
ASME V&V 10. Standard for Verification and Validation in Computational Solid Mechanics. The American Society of Mechanical Engineers.
ASME V&V 10.1. An Illustration of the Concepts of Verification and Validation in Computational Solid Mechanics. The American Society of Mechanical Engineers.
ASME VVUQ 10.2. The Role of Uncertainty Quantification in Verification and Validation of Computational Solid Mechanics Models. The American Society of Mechanical Engineers.
ASME V&V 20. Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer. The American Society of Mechanical Engineers.
ASME V&V 40. Assessing Credibility of Computational Modeling Through Verification and Validation: Application to Medical Devices. The American Society of Mechanical Engineers.

1.3.2 Other Industry Publications

AIAA-G-077 (1998). Guide for Verification and Validation of Computational Fluid Dynamics. American Institute for Aeronautics and Astronautics.
Anderson, M. G., and Bates, P. D. (Eds.) (2001). Model Validation — Perspectives in Hydrological Sciences. John Wiley and Sons.
Bossel, H. (1994). Modeling and Simulation (1st ed.). A. K. Peters.
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2 MOTIVATION TO HARMONIZE ASME VVUQ RESOURCES

2.1 Need for Trusted Models

The increasing use of computational models and simulations (M&S) across a broad range of scientific disciplines and engineering applications is a testament to how well advancements in M&S have succeeded in harnessing the exponential growth of computational power. It also underscores the vast potential for growth of M&S and their applications as they catalyze emergent and as yet unrecognized opportunities. However, along with the seemingly boundless upside, such rapid growth brings with it risks stemming from applying models without recognizing their inherent limitations. In an absolute sense, as attributed to George Box, "All models are wrong, but some are useful"[1] and it is in the discipline of VVUQ where a model's "wrongness" and "usefulness" are studied.

The goal of VVUQ is to provide a systematic and objective method that can be used to determine the extent to which M&S can be trusted for some given purpose. While the resources spent performing VVUQ are typically driven by the consequences of the simulation, the VVUQ activities are generally the same for most models. Further, it is vital to define for what uses the model should and should not be trusted. This task becomes increasingly important as many models are reused or repurposed for new applications. In summary, as the reliance on computational M&S increases, there must be a corresponding emphasis on alleviating the potential adverse consequences by assessing the reliability that M&S can be trusted for their context of use (intended use).

2.2 ASME VVUQ Committees

(a) ASME has led the development of standards for methods and procedures for VVUQ since 2001. The charter of the Verification, Validation, and Uncertainty Quantification in Computational Modeling and Simulation Committee (VVUQ Committee) is, "Coordinate, promote, and foster the development of standards that provide procedures for assessing and quantifying the accuracy and credibility of computational models and simulations." Currently, the VVUQ Committee has the following seven subcommittees:

(1) VVUQ 10 Subcommittee — Verification, Validation, and Uncertainty Quantification in Computational Solid Mechanics

(2) VVUQ 20 Subcommittee — Verification, Validation, and Uncertainty Quantification in Computational Fluid Dynamics and Heat Transfer

(3) VVUQ 30 Subcommittee — Verification, Validation, and Uncertainty Quantification in Computational Nuclear System Thermal Fluids Behavior

(4) VVUQ 40 Subcommittee — Verification, Validation, and Uncertainty Quantification in Computational Modeling of Medical Devices

(5) VVUQ 50 Subcommittee — Verification, Validation, and Uncertainty Quantification of Computational Modeling for Advanced Manufacturing

(6) VVUQ 60 Subcommittee — Verification, Validation, and Uncertainty Quantification of Modeling and Simulation in Energy Systems

(7) VVUQ 70 Subcommittee — Verification, Validation, and Uncertainty Quantification of Machine Learning

[1] Box, G. E. P. (1979). "Robustness in the Strategy of Scientific Model Building." In R. L. Launer and G. N. Wilkinson (Eds.), Robustness in Statistics (pp. 201–236). Academic Press.

(b) The subcommittees' activities include producing standards that establish the theory, methods, and application of VVUQ to solve engineering problems. While each standard is written from a given perspective (i.e., discipline or application), each subcommittee is encouraged to produce broadly applicable standards that are relevant across multiple engineering communities. To date, the following documents have been published:

(1) ASME V&V 10, Standard for Verification and Validation in Computational Solid Mechanics. This standard provides a common language, a conceptual framework, and general guidance for implementing the processes of computational model VVUQ focusing on the computational solid mechanics community.

(2) ASME V&V 10.1, An Illustration of the Concepts of Verification and Validation in Computational Solid Mechanics. This standard provides an example of the key elements from the VVUQ process described in ASME V&V 10.

(3) ASME VVUQ 10.2, The Role of Uncertainty Quantification in Verification and Validation of Computational Solid Mechanics Models. This standard provides an overall description of the role of uncertainty quantification in the VVUQ process.

(4) ASME V&V 20, Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer. This standard provides a procedure to estimate the modeling error of a quantity of interest determined by a mathematical model used to simulate the same physical reality, while accounting for experimental, numerical, and input uncertainties.

(5) ASME V&V 40, Assessing Credibility of Computational Modeling Through Verification and Validation: Application to Medical Devices. This standard provides a method to assess the credibility of computational modeling for applications related to medical devices. While the examples in this standard are specifically written for the medical device community, ASME V&V 40 may be applied to the M&S activities in other industries.

2.3 Synergies Across M&S Communities

While the subcommittees focus on applications of VVUQ methods for their specific disciplines, they share a common goal of consolidating the best practices to generate evidence necessary and sufficient to justify using models for defined contexts of use. Although parallel development efforts require minimizing overlap of efforts and redundancy, they also provide the opportunity to adapt and apply methods from other technology domains. ASME has focused on publishing standards for specific communities through their subcommittees, but also publishes standards that span multiple communities. This Standard represents a step toward harmonizing those communities by providing a common vocabulary.

2.4 Other VVUQ Activities

ASME provides forums to promote synergies across M&S communities. This includes publishing the *Journal of Verification, Validation, and Uncertainty Quantification* (JVVUQ) and hosting a symposium annually. JVVUQ[2] disseminates original research in the development and application of methods for performing code and solution (calculation) verification, simulation validation, and simulation and experimental uncertainty quantification. The VVUQ symposium[3] brings together engineers and scientists from all disciplines that use computational M&S to discuss and exchange ideas and methods for verification of codes and solutions, simulation validation, and assessment of uncertainties in mathematical models, computational solutions, and experimental data.

3 TERMINOLOGY

This section contains key terms and definitions that are commonly used, but not always consistently defined, within the computational modeling and simulation (M&S) community. The goal is for this section to serve as a common glossary to represent the ASME VVUQ philosophy applied to the breadth of disciplines covered by the subcommittees. The terminology is divided into categories based on the high-level stages involved in the modeling process.

(a) Purpose and Scope
(b) Model Development
(c) Verification and Validation
(d) Uncertainty Quantification
(e) Credibility Assessment

The flow is nominally presented in the order that a developer or analyst might encounter the terms in the process of model development and application. Each term is accompanied by key points of clarification for increased understanding and consistent communication.

[2] https://journaltool.asme.org/home/JournalDescriptions.cfm?JournalID=29&Journal=VVUQ
[3] https://event.asme.org/V-V

3.1 Purpose and Scope

The purpose and scope of M&S defines not only what is being modeled but also why. Why is the simulation being performed? What information is expected to be gained by M&S? What phenomena need to be simulated to obtain that information? Will the M&S results play a primary or secondary role in supporting a decision? What are the consequences if a simulation is not sufficiently accurate? Understanding these concepts is necessary to fully articulate the purpose of the model and the limitations of its scope.

3.1.1 Question of Interest. The question of interest is the specific question, decision, or concern that is being addressed.

The question of interest is not solely focused on the M&S activities, but instead is the overall project goal. It is the question that scientists, engineers, or managers must answer. Often, at a high level, the question of interest is a technical decision (e.g., is the bridge safe, does the product satisfy requirements), but it may also be a question related to understanding (e.g., how quickly a virus can spread). However, the question of interest may be more nuanced and specific to the application.

A clear grasp of the question of interest is essential for achieving the purpose of the simulation. M&S is performed for a reason. It is used to help answer a question in science or engineering. Sometimes, M&S provides the entire answer, but often M&S is only part of the answer to a larger question.

Inherent in answering the question of interest is understanding the consequences of answering the question incorrectly. If part of the answer involves M&S, then we must consider the consequences of errors in the M&S. These consequences are often directly correlated to the VVUQ effort, with more serious consequences usually having a larger investment in VVUQ.

3.1.2 Context of Use. The context of use,[4] or context of model use, is the specification of the role and scope of the computational model used to address the question of interest.

The context of use, or intended use, should include a detailed statement of what will be modeled and how the outputs from the computational model will be used to answer or inform the question of interest. This context of use defines how important the simulation is in answering the question of interest and drives the rigor of the VVUQ effort.

One way to understand the role of the model is to ask, "what if we could not use the model in answering the question of interest?" Would not having the model make answering the question impossible? Much harder? Or would it have little impact? Understanding how much we rely on the model results defines the model's role in answering the question of interest. For example, in situations where there will be proof testing, the model's role may be smaller, as the question of interest will be greatly informed by the results of those tests. However, if such testing is not available, the model's role may greatly increase as the question of interest could be only answered by the model's results.

One way to understand the scope of the model is to ask, "what evidence is the model providing in answering the question of interest?" Primarily this focuses on phenomena that are being modeled, over what ranges they are being modeled, and to what level of detail they are being modeled. Understanding the evidence generated from model results defines the model's scope in answering the question of interest.

When a simulation is determined to be credible (i.e., it is trusted), it is only for a specific context of use. A change in that context of use would impact the credibility determination. If the model's role were increased or decreased, the VVUQ requirements for credibility would also likely increase or decrease correspondingly. Similarly, if the model's scope was changed, this would likely result in a change to the VVUQ activities that would need to be performed to determine the model's credibility. Hence, the credibility determination is based on a specific context of use and any change in that context of use would require a new determination.

While the context of use is defined in terms of a computational model and the resulting simulations from that model, empirical data (e.g., experiments) also have a context of use. Like simulations, data from an experiment found appropriate for one context of use may not be found appropriate for another.

3.1.3 System. A system is an entity, environment, object, phenomenon, process, or combination thereof.

The definition of "system" is intentionally broad such that it includes all possible uses. A specific system is defined by its boundaries, which specify what is considered internal to the system and what is considered external. However, those boundaries, and systems in general, are a conceptual construct.

While the term "system" will be used with this broad meaning in this Standard, when used in a specific field the term often takes on a more detailed meaning. For example, in certain subgroups of the M&S community, the term may have a more restricted definition (e.g., a system may mean a quantity of matter, volume in space, or a manufacturing process).

3.1.4 System Behavior. System behavior is the action, work, or response of a system.

[4] The term "context of use" is commonly abbreviated as "COU."

The system behavior can be thought of as the "transfer functions" that change the state of the system. For physical systems, the system behavior is defined by the laws of physics. In scientific computing, one of the main goals is to generate a computational model of the system that has the same system behavior as a corresponding physical system.

3.1.5 System State. A system state is the collection of values of the parameters or variables that are the result of the system behavior.

The initial condition is the system state at the beginning of a scenario. The boundary conditions define the values of the system state at the boundaries of the system and generally change with time during a scenario. The final condition is the system state at the end of a scenario. Thus, a scenario consists of the system state at the initial condition, the system state at the final condition, and all system states in-between.

3.1.6 Quantity of Interest. A quantity of interest[5] is a quantity that provides important information about the system state.

System states are associated with large sets of numerical values (i.e., quantities). While all of these quantities may be important, there are generally a subset of these quantities that are of primary interest and will be used to help answer the question of interest. The quantity of interest can be almost any quantity, such as a specific variable (e.g., the temperature of the wall), a specific variable over a specific range (e.g., the temperature at the midplane of the wall), or a single value of a specific variable (e.g., the maximum temperature of the wall). A quantity of interest applies to experiments, simulations, and the underlying system of interest.

There are a set of terms closely associated with quantities of interest. However, it is difficult to determine whether these terms are truly synonyms or have a nuanced difference. This is because authors using the terms seem to have different opinions. Potential synonyms include system response quantity (SRQ), response quantities of interest, and figure of merit (FoM).

3.2 Model Development

Model development begins with the selection of the system and the specification of the system behavior(s) of interest. The focus of model development is to develop a set of solvable mathematical equations that describe the system behavior (i.e., physics). This system of equations can then be used to make predictions of the system behavior in scenarios of interest.

3.2.1 Model. A model is a representation of system behavior.

The purpose of a model is to provide an estimate of system behavior. As with the definition of "system," the definition of a "model" is intentionally broad such that it includes all possible uses. While this broad definition also accounts for physical models (e.g., airfoil in a wind tunnel), in the M&S community the term is usually associated with a conceptual, mathematical, or computational model and may act as shorthand for any of these. In the VVUQ community, when the term "model" appears without a qualifier, it generally refers to the computational model.

3.2.2 Conceptual Model. A conceptual model is a collection of assumptions and process descriptions representing a specific system behavior.

By definition, a conceptual model is a concept. As with any concept, it can range from something as unarticulated as an analyst's understanding of a system to something as concrete as a formal abstraction that describes the most important assumptions, approximations, and environment that govern the system behavior. Being able to state which issues or physical processes are ignored or approximated minimizes ambiguity in the development of the mathematical model, computational model, and validation experiments.

3.2.3 Mathematical Model. A mathematical model is the collection of mathematical relationships needed to describe the conceptual model.

The mathematical model includes all necessary mathematical structures (e.g., equations, regression models, neural networks) needed to completely describe the conceptual model. The mathematical structures are chosen such that they reflect the assumptions in the conceptual model. However, the use of a specific mathematical structure may introduce additional assumptions that were not part of the conceptual model.

3.2.4 Computational Model. A computational model is the representation of the mathematical model such that it can be executed on a computer.

While the mathematical model often contains the most complete description of a system behavior, it may not be possible or practical to compute the results from that model. Therefore, an altered version of the mathematical model is used that is easier to compute and is called the computational model. The computational model is typically a set of instructions (e.g., algorithm, computer code), which can be executed on a computer. Representing the mathematical model on a computer may introduce additional assumptions (e.g., assuming the discrete equations provide the same results as the continuous versions) that were not part of the mathematical or conceptual models. Furthermore,

[5] The term "quantity of interest" is commonly abbreviated as "QOI."

when performing a simulation for a specific question of interest and a specific context of use, the focus is on a specific computational model and not the universe of models that could be created within a computer code (e.g., analysis software). It is important for the analyst to specify what is defined as the computational model such that VVUQ may be performed consistently with the context of use of the model.

3.2.5 Simulation. A simulation is the act of executing the model.

In practice, the term "simulation" is often used to refer to both the act of executing the model and the results generated by executing the model. This Standard has separated these two using the term "simulation" alone for the former and "simulation results" for the latter. However, these terms are often used interchangeably in the literature. For example, the statements "The simulation shows …" and "The simulation results show …" are both common. It is possible to have simulations that result from executing a conceptual model (i.e., conceptual simulations) or a mathematical model (i.e., mathematical simulations). However, in this Standard, as in most VVUQ literature, the term "simulation" is used as shorthand for a computational simulation that results from executing the computational model.

3.2.6 Simulation Results. The simulation results are the system states calculated by executing the computational model.

The simulation results include all quantities that are calculated by the computational model. In general, there are specific calculated quantities that are of more interest than others; those are defined as quantities of interest. For example, the simulation results may include every temperature calculated by a computational model along a plate, while the quantities of interest may include only the calculated temperature at the end of the plate.

3.3 Verification and Validation

Once the computational model has been developed, there needs to be some assurance that the model can predict the system behavior to a sufficient accuracy. This assurance relies on performing two key assessments: verification and validation. Verification is performed to compare the computational model to the mathematical model. Validation is performed to compare the predictions of the computational model with empirical data.

3.3.1 Empirical Data. Empirical data are the measured behaviors of a physical system with associated uncertainties.

Measured behaviors of physical systems are often thought of as experimental measurements. This Standard uses the broader term "empirical" to include all data obtained from real-world systems, including data from sources generally not considered to be experiments (e.g., human populations, manufacturing, in-service systems). Empirical data include data taken directly from instruments, quantities derived from those instruments (e.g., through data reduction models), observations, user experience, etc.

As discussed in para. 3.4, uncertainty quantification is an important element in determining simulation credibility. Not reporting uncertainties associated with empirical data disregards uncertainties that exist.

3.3.2 Referent. A referent is a reference value (or set of values) against which simulation results or empirical data are compared.

The ideal referent is the true value, but only in special situations is the true value known. For example, a true value may be known during some portions of code verification and during some types of instrument calibration. If the true value is not knowable, then the justification for the referent should be given. Referents for verification include the results from analytic solutions, manufactured solutions, and numerical benchmark solutions. Referents for validation include measurements and associated uncertainties. These measurements (e.g., empirical data) often come from validation experiments or in-use systems.

3.3.3 Verification. Verification is the process that establishes the mathematical correctness of the computational model with respect to a referent.

In general, there are many verification activities that are associated with M&S, including data verification, input verification, procedural verification, code verification, and solution verification. This Standard focuses on code and solution verification. The other verification processes, while important, are not formally defined in this Standard.

3.3.3.1 Code Verification. Code verification is the process of determining that the mathematical models are correctly implemented in the computer code and of identifying errors in the software.

Code verification is an error identification process through the evaluation of whether the computational model is consistent with the underlying mathematical model. This process begins with comparing the results from the computational model to exact solutions of the mathematical model. Code verification relies on having a robust software quality assurance program to minimize the occurrence and severity of "bugs" in the software. Techniques for code verification include the use of analytical solutions and the method of manufactured solutions.

3.3.3.2 Solution Verification. Solution verification is the process of determining the accuracy of a particular numerical solution relative to an estimate of the exact solution of the computational model.

Solution verification (i.e., calculation verification) is an error estimation process. The same computational model can have different results introduced by sources such as discretization, iteration, and computer precision. For example, we would get different results if we had access to a computer with infinite resources compared to the results we obtained from our computer with finite resources. We use solution verification to determine how much our computational results deviate from those results we would obtain if we had access to a computer with infinite resources (i.e., the exact solution of the computational model). Solution verification may need to be performed for each use of a computational model as the solution verification results may vary with changes to initial conditions, boundary conditions, gradients of the dependent variables, and modeling options.

We perform code verification before solution verification because we want to ensure that the exact solution of the computational model is equivalent to the exact solution of the mathematical model. Therefore, it is only if code verification has been performed that solution verification provides the accuracy of a particular numerical solution relative to an estimate of the exact solution of the mathematical model.

3.3.4 Validation. Validation is the process of determining the degree to which a model represents the empirical data from the perspective of the context of use.

Validation provides evidence of how closely the output from the model matches observations of a physical system. This assumes that the physical system (e.g., airfoil in a wind tunnel) captures the relevant physics of the real-world system of interest in its operating environment (e.g., airplane in flight). This process involves comparing the simulation results to empirical data to estimate the modeling error and includes an assessment of all the uncertainties in both the empirical data and the simulation. In general, empirical data comes from historical experiments, dedicated validation experiments, or measurements of the system in use. The use of dedicated validation experiments facilitates key experimental quantities to be measured as completely and accurately as possible. However, the experimental system behavior may be different from the real-world system behavior. On the other hand, while in-use systems have the same behavior as the real-world system, the key experimental quantities may not be measured as completely or as accurately.

The process of validation is initiated after both code verification and solution verification have been performed. This ensures the mathematical correctness of the model before estimating the errors in the model's representation of the physics. The primary outcome of validation is an assessment of the modeling error for a specific condition or set of conditions and not a pass-fail statement. That assessment should be a quantitative measure(s) of the level of agreement between empirical data and simulation results. Acceptance of a model can lead to claims of a "validated model"; however, no computational model should be considered broadly "validated." Instead of saying "the model is validated," it is better to say "the model is valid to predict the quantities of interest (X1, X2, X3 …) each with a specified uncertainty (U1, U2, U3) in the context of use (Y)."

It should be noted that comparison of simulation results with results from other computational models (e.g., code-to-code comparison, direct numerical simulation) is not validation.

3.3.5 Validation Metric. A validation metric is a mathematical measure that quantifies the level of agreement between simulation results and empirical data for a quantity of interest.

The primary outcome of validation is a quantitative measure(s) of the level of agreement between empirical data and simulation results. The validation metric is the mathematical formulation through which that quantitative characterization is obtained. A quantitative (as opposed to qualitative) comparison ensures this characterization is objective. The specification and use of validation metrics are a critical element of the validation activities, as the results from the validation metric calculation will differ depending on the metric chosen. It is important to choose a metric in which the results are meaningful to the context of use and can be readily understood by the analyst as well as the subsequent decision maker.

3.4 Uncertainty Quantification

In the context of verification and validation, uncertainty quantification is the mathematical assessment of the uncertainties that arise from all sources of uncertainty in the simulation, experimentation, and real-world systems and processes.

3.4.1 Error. Error is the difference between a measured or calculated value and the true value or its proxy.

The terms "error" and "accuracy" are often used in a similar manner, in that "error" is used to stress how far apart the measured value or calculated value is from the true value while "accuracy" is used to stress how close the measured value or calculated value is to the true value. While we would like to use the true value when calculating an error, the true value is often unknown and may be unknowable. Therefore, we often must use a proxy to determine the error. Both the true value and its proxy are considered as referents. Finally, an error could be impacted by both systematic and random effects.

3.4.2 Uncertainty. Uncertainty is the recognition of the imperfect knowledge about a system or quantity.

Uncertainty is generally attributed to incomplete information, incomplete understanding, or inherent variability. Epistemic uncertainty is defined as incomplete information or understanding. Aleatory uncertainty is defined as inherent variability, often expressed using probability distributions. Uncertainty can contain contributions from both aleatory and epistemic sources. For example, measurement uncertainty, which is defined as the lack of exact knowledge of the value of the measured quantity, often has both aleatory and epistemic components.

3.4.3 Uncertainty Quantification. Uncertainty quantification is the process of generating and applying mathematical models to provide a measure of uncertainty in the empirical data or simulation results.

Uncertainty Quantification (UQ) requires models that represent the uncertainty in the value of specific quantities. This uncertainty can result from inherent variability but may also result from lack of knowledge. The main aspect of UQ is the characterization of uncertainty; it may include propagating that uncertainty. Characterization of uncertainty focuses on representing or modeling the uncertainty in a given quantity. An example of characterization is collecting sample data and estimating statistics or fitting probability distribution models to those data. Propagation of uncertainty focuses on determining the impact of uncertainty on the quantities of interest. Examples of propagation methods include Monte Carlo sampling and Taylor Series sensitivity analysis.

3.5 Credibility Assessment

The final step before using a model is determining if the computational model can be trusted to make predictions of the system behavior for its context of use. This determination is based on evidence that has been collected during the VVUQ activities for the specific context of use. To properly evaluate the credibility of a model, the credibility of the empirical data and referents must also be evaluated.

3.5.1 Applicability. Applicability is the relevance of the evidence from the verification, validation, and uncertainty quantification activities to support the use of the computational model for a context of use.

Applicability assessment is the process whereby we determine if the VVUQ activities performed and the evidence generated from those activities are relevant for the context of use of the model. This evidence is the available body of facts or information, which demonstrates that the computational model can be trusted for its context of use.

Frequently, applicability examines questions relating to validation and context of use: How similar is the system in which the model will be applied to the system in which empirical data was obtained? How do the quantities of interest used in the validation activities relate to the quantities of interest of the context of use? However, applicability also considers questions relating to verification and UQ: Which portions of the code were exercised in code verification and which portions will be used when making predictions? Over which range were the portions of the code exercised? How relevant is the UQ for the anticipated conditions of the context of use?

3.5.2 Predictive Capability. Predictive capability is the anticipated accuracy of the computational model for conditions where no empirical data are available.

During validation, the model's prediction and its uncertainty are compared to empirical data and its uncertainty typically using a validation metric. However, the validation data is often obtained from a physical system that is different from the real-world system of interest for which the model will be used to make future predictions. Thus, the model's prediction uncertainty for the real-world system of interest (where no empirical data exists) is often greater than the uncertainty observed during validation. The predictive capability is generally based on the relative size and influence of the quantified uncertainties from the verification and validation processes. However, predictive capability must also address how those uncertainties may change, and new uncertainties may appear when considering the real-world system. It is emphasized that the model's predictive capability is based on a diverse set of contributing uncertainties, and as such relies on engineering judgment based on the accumulated evidence during the VVUQ process.

3.5.3 Credibility. Credibility is the trust, established through the collection of evidence, in the predictive capability of a computational model for a context of use.

Credibility assessment is a judgement as to whether a model can be trusted to support answering the question of interest given on the evidence gathered during verification and validation along with an assessment of the uncertainties. Such judgments are made by multiple individuals throughout the model assessment process and consider the applicability of the evidence to the context of use, as well as other factors that could affect the model's prediction of the system of interest (e.g., the experience of the analysts, the maturity of the M&S process followed, the significance of the simulation, adverse consequences from trusting the simulation, uncertainties in the system). Credibility assessment commonly results in a binary determination of either "yes — the model can be trusted" with some level of uncertainty or "no — the model cannot be trusted" for its context of use.

4 ELEMENTS OF VERIFICATION, VALIDATION, AND UNCERTAINTY QUANTIFICATION

The following figures provide a graphical summary of the terminology and concepts defined in this document:

(a) The terms associated with purpose and scope are given in Figure 4-1.
(b) The terms associated with model development are given in Figure 4-2.
(c) The terms associated with verification and validation are given in Figure 4-3.
(d) The terms associated with uncertainty quantification are given in Figure 4-4.
(e) The terms associated with credibility assessment are given in Figure 4-5.

Figure 4-1
Purpose and Scope

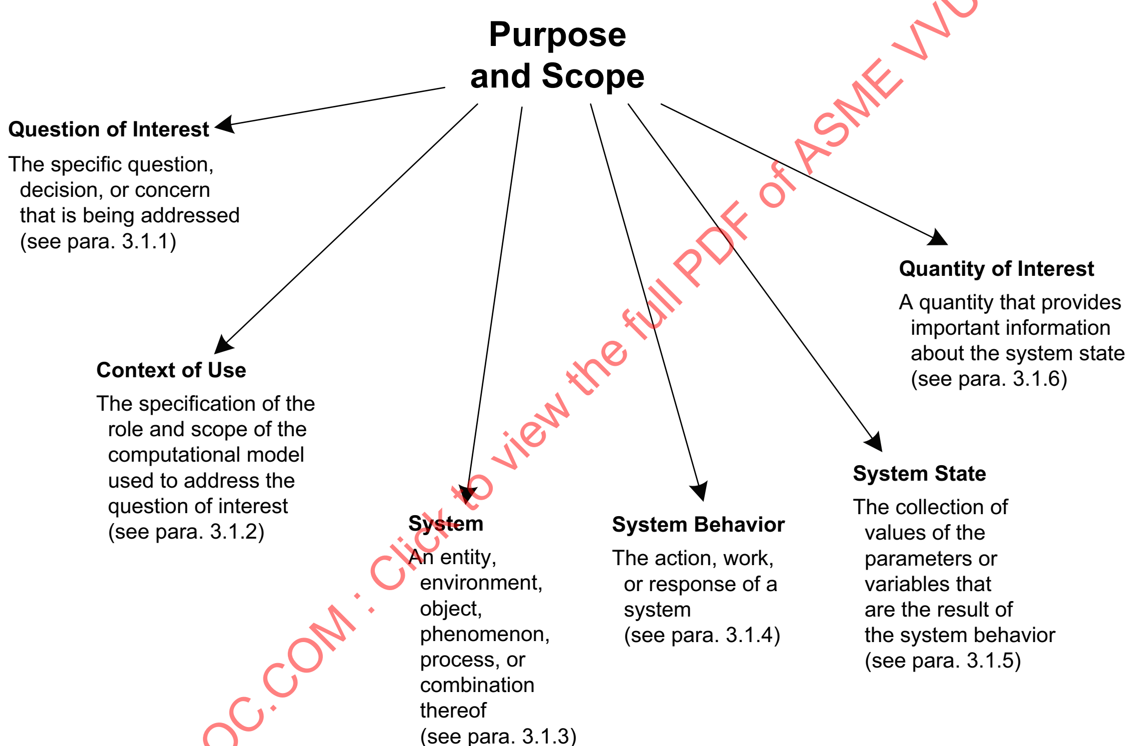

Figure 4-2
Model Development