CALIBRATION IN COMPUTATIONAL MECHANICS

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Background

The issue of "calibration" has been addressed in several previous documents, as documented in the Appendices. The current discussion is derived from the AIAA Guide, whose discussion of Calibration is included here as Appendix 1. Appendix 2 is the relevant section of Patrick Roache's book, which provides extensive insight into the view of Calibration from the perspective of Computational Fluid Dynamics.

The Calibration Process

Ideal verification and validation procedures for simulations involving complex material processes or multidisciplinary engineering systems routinely become impractical. For example, when all of the important physical modeling parameters are not known a priori, some of the parameters are considered adjustable. Similarly, when mesh convergence is not obtained, the results may be accepted "as-is", or adjustments must be made to improve agreement with the experimental data. These types of activities are termed "calibration"; the AIAA Guide definition is used here verbatim:

> • **Calibration**: The process of adjusting numerical or physical modeling parameters, components, or aspects of the computational model for the purpose of implementing a computational model or improving agreement with experimental data.

Calibration is an integral and pervasive part of the model development process in computational mechanics, particularly in CSM. The definition of Calibration describes a "process of adjusting" that is both explicit and implicit; many forms of Calibration are not readily recognized or intended by the analyst. Examples of Calibrations include, but are not limited to:

- Acceptance of constitutive models, and tuning of constitutive model parameters,
- Implementation of boundary conditions,
- Use of sub-models (e.g., springs, joints), and their avoidance (e.g., simple continuity where a weld exists),
- Lack of mesh convergence,
- Employment of a deterministic approaches to stochastic problems,
- Implementation of "artificial viscosity" to approximate discontinuous shock fronts as steep but continuous fronts.

Although it is widely accepted that Calibration plays a significant role in computational mechanics - particularly in CSM - the community has not reached consensus on the components of Calibration presented above. In particular, the inclusion of "acceptance of non-converged meshes" can raise the objection that such an inclusion implies approval of "bad science". Indeed, the scientific foundation of computational mechanics is based, in large part, on the assumption of mesh convergence. In practice, however, true mesh convergence is rarely demonstrated on simulations of practical, complex systems. Exceptions include some applications of CFD, a field more mature than CSM in terms of V&V, as evidenced by more stringent peer-reviewed publication requirements.

An "inclusive" approach to Calibration is advocated here that acknowledges that simulations lacking mesh convergence will continue to be the norm well into the future. Instead of developing guidelines for V&V that apply only to converged mesh simulations (a vanishingly small segment of the simulation world), the proposed approach is to document the consequences of individual Calibrations (including lack of mesh convergence). Only by doing so will practitioners and managers have the information available to them to assess the usefulness of various approaches to computational mechanics.

Calibrations enforce many practical limitations on simulation by constraining simulation validity, thereby reducing predictive capability. Stated differently, Calibrations affect "how far" from the existing experimental database one can make a prediction and still retain an acceptable level of confidence in the prediction. Although Calibrations are routine, their effects are rarely quantified. For example, it might be expected that lack of mesh convergence so severely constrains model validity that predictive capabilities are practically eliminated (thereby practically negating the usefulness of the model). However, this conclusion has not yet been established.

Simulation in the absence of quantification and documentation of the effects of Calibration is analogous to the acceptance of unquantified experimental data.

Summary.

Calibration is pervasive in computational mechanics - particularly CSM - and is usually implicit within the overall model development process. Proper V&V of a model, and any hope for use of the model in a predictive capacity, demand that the degree of Calibration be quantified and documented.

Appendices – Discussions of Calibration in the Literature

Appendix 1 – AIAA, "Guide for the Verification and Validation of Computational Fluid Dynamics Simulations" - 2.2 Verification and Validation, and 4.2 Calibration

In simulations involving complex flow physics or multidisciplinary engineering systems, strict validation procedures commonly become impractical. For example, when all of the important physical modeling parameters are not known a priori, some of the parameters are considered adjustable. Or when grid-resolved solutions are not attainable because of the computer resources needed for the simulation, adjustments must be made to improve agreement with the experimental data. When these types of activities occur, the term calibration more appropriately describes the process than does validation.

The quantification of prediction increments is the most common use of modeling and simulation in engineering. This conservative approach provides incremental changes in complex systems and processes so that a wide variety of modeling and simulation shortcomings can be tolerated without unacceptable risk. For example, the difference between the design expectation and actual performance of a fluid dynamics system, say an aircraft or a turbopump, is a measure of the uncertainty and error inherent within the simulation. Once the uncertainty and error have been estimated, the same design simulation tools are used in the same manner to estimate the performance of other similar systems operating in a comparable environment. This is commonly done either by adding the known uncertainty and error to the simulated performance value, or by adjusting for various elements of the simulation so that the computational results agree with the measured results. Adjustment activities are commonplace in complex CFD simulations and are conceptually different from activities associated with the validation process. In effect, adjustment activities comprise a different process, which we refer to by the term calibration.

- Calibration: The process of adjusting numerical or physical modeling parameters in the computational model for the purpose of improving agreement with experimental data.

Calibration is not "the process of determining the degree to which a model is an accurate representation of the real world." Calibration is primarily directed toward improving agreement of computational results with existing experimental data, not determining the accuracy of the results. Because of constraints in fiscal budgets and computer resources, or because of incomplete physical modeling data, calibration is commonly an appropriate process when compared to validation. The distinction between calibration and validation is not always crisp or easily recognizable in many situations. However, attempts should be made to recognize when calibration is exercised because it directly impacts the confidence in predictions from the CFD model. Stated differently, calibration affects "how far" from the existing experimental database one can make a prediction and still retain an acceptable level of confidence in the prediction. Calibration does not generate the same level of predictive confidence as validation.

The need for calibration commonly arises when there is uncertainty in the modeling of complex physics processes and also when there are incomplete or imprecise measurements in the experiments. Situations in which physical modeling parameters are commonly adjusted are found in the computation of turbulent combusting flow, multiphase flows, and flows with strong coupling to other physical processes, such as acoustics, structural dynamics, and radiation transport. For example, consider the use of the Reynolds-Averaged Navier Stokes equations in computing turbulent reacting flow with finite rate chemistry. It is common practice to adjust chemical reaction rates so that improved agreement with experimental data is obtained. Another example is the adjustment of unmeasured or poorly characterized experimental parameters (e.g., boundary conditions) in comparisons of computations with experimental data. Incomplete or imprecise experimental data are often viewed as opportunities to adjust parameters in the code when making comparisons with experimental data. This type of physical parameter adjustment activity is similar to the highly developed technique of parameter identification used in many other disciplines. For example, in structural dynamics, mechanical joint stiffness and joint damping are clearly identified as physical modeling parameters that are optimally estimated in simulation comparisons with experimental measurements of structural modes. Formal parameter identification procedures clearly recognize the calibration nature of the analysis.

How CFD calibration activities impact confidence in predictions (i.e., the accuracy of future computational results) is very difficult to determine and is presently beyond current technology. Similarly, the issue of assessing the accuracy of predictions is usually complicated by the lack of grid or time-step convergence in the calibration computations. It is common engineering practice to use the results of CFD simulations for complete systems and subsystems applications for which grid- resolved solutions are not attained - possibly far from being resolved. Indeed, benchmark cases with complex physics, particularly three-dimensional simulations, may not have grid-resolved solutions. When physical modeling parameters are determined based on solutions on grids that are clearly under-resolved, the activity should be considered as part of the calibration. The calibration nature of this type of activity is recognized if the physical modeling parameters are readjusted based on solutions obtained on finer grids. The calibration nature of such an activity should also be recognized if grid refinement is stopped when generally good agreement is obtained with the important experimental measurements; in other words, if further refined grids show degraded agreement with the experimental data.

As mentioned earlier in this section, some of the subtleties of calibration as compared to validation are highlighted in order to further the understanding of each process. Also, improved understanding of calibration and validation will aid in developing future methods for quantitatively estimating confidence in predictions for complex systems.

Appendix 2 – Patrick Roache, “Verification and Validation in Computational Science and Engineering” - 2.12 CALIBRATION AND TUNING

The term “Calibration” is used with more latitude than Verification, Validation, or Confirmation.

I prefer to use the term “Code Calibration” to mean the adjustment of parameters needed to fit experimental data, e.g. the 6 closure coefficient values necessary for two-equation turbulence models. Some other CFD practitioners agree, e.g. Marvin (1995), who gives the following description.

"Code parameters such as turbulence models may need to be adjusted to accommodate applications for geometries and conditions outside the envelope of their original validation. Experiments intended to support this activity can be referred to as Calibration experiments." (Marvin, 1995)

As an example of Calibration, Marvin (1995) cites the work of Coakley and Huang (1992) in which basic k-ε and k-ω turbulence models are [rationally] corrected for compressibility and length scale, vastly improving the experimental agreement for surface pressures and heating rates on an ogive-cylinder-flare body at Mach number 7. Importantly, the good agreement was maintained for other hypersonic experiments on shock interactions.

Likewise, Mehta (1996) is clear that “Calibration is not the process of determining the level of accuracy or credibility, but is the process of obtaining correction factors.” Consistent with Marvin and with Mehta, Porter (1996) notes the dictionary definition of Calibration: “to standardize by determining the deviation from a standard so as to ascertain the proper correction factor.” Rizzi and Vos (1996) are also consistent with this view. “Calibration is the process of Tuning or Calibrating a code with a particular fluid dynamics model to improve its prediction of global quantities for realistic geometries of design interest. This has to be done because there is no universal turbulence...”

However, other colleagues assure me that the term Calibration is used in experimental studies just as a means of ascertaining accuracy, or more properly of determining the inaccuracy, e.g. of a pressure probe or a wind tunnel test section flow. (Oberkampf, 1994 notes that the term “Validated” is never used for an experimental ground test facility because it would be a misnomer. Rather, facilities are Calibrated.) If extended to codes as in Aeschliman et al (1995), this definition, in my mind, makes “Code Calibration” almost indistinguishable from Validation, or perhaps Validation for a more restricted range of parameters. Indeed, Porter (1996) gives the definitions adopted by a NASA *ad hoc* committee.

- *Validation*: “comparison with experiment to verify [sic] the ability to accurately model over a range of parameters [sic].
- *Calibration*: comparison with experiment to provide a measure of the ability to predict specific parameters [sic].”

Even if we ignore the unfortunate use of term “verify” in a common- language (rather than technical context) sense, and overlook the use of “parameters” in two different senses (the first as an input parameter, the second as solution value), these NASA definitions still offer little distinction, with Validation involving a range of parameters but Calibration involving specific parameters. See also Bradley (1988).

Aeschliman et al (1995) use (as do others) the triplet “Code Verification, Calibration, and Validation” or VCV and give this description of Calibration. “We loosely interpret code ‘Calibration’ to mean a code’s ability to reproduce valid data (not exclusively experimental) over a specified range of parameters, for some geometry, without necessarily assessing the overall correctness of all of the physical models employed. We consider Calibration to be a less-demanding element of Validation, and is addressable experimentally by the same methods." For CFD, I prefer Marvin's (1995) description above.

Bradley (1988) summarized the substance of a NASA study of a process for CFD Validation, and distinguished code Validation from Calibration as follows. (The quote is from Marvin, 1995.)

"CFD code Validation: Detailed surface and flowfield comparisons with experimental data to verify the code's ability to accurately model the critical physics of the flow. Validation can occur only when the accuracy and limitations of the experimental data are known and thoroughly understood and only when the accuracy and limitations of the code's numerical algorithms, grid density effects, and physical basis are equally known and understood over a range of specific parameters. CFD code Calibration: The comparison of CFD code results with experimental d~ta for realistic geometries that are similar to the ones of interest, made to provide a measure of the code's ability to predict specific parameters that are of importance to the design objectives without necessarily verifying that all of the features of the flow are correctly modeled."

Note that the term "Calibration" also has traditionally been applied to the empirical adjustment of constants in a theoretical analysis, as in Bradley (1988). Marvin (1995) goes on to state that "During the intervening years since these definitions were formulated [1988], it has been argued that the definition of Validation is too restrictive, especially for the complex applications associated with realistic geometries. Nevertheless, NASA has maintained the definition as a goal of its Validation process."

In my opinion, definitions or descriptions should avoid attempts to enforce levels of accuracy, which descriptions are inevitably vague anyway (e.g., "detailed," "thoroughly understood," etc.) and leave these qualifications simply to the evaluation of the thoroughness of the Validation (or invalidation). Also, as I have noted earlier, assessment of "grid density effects" is not a code property per se, but rather a property of the particular code application, i.e., part of Verification of a particular calculation rather than Verification of a code.

Many people simply equate Calibration with the adjustment of parameters that is called "Tuning," and often "somewhat without scientific justification" (Mehta, 1996)." In addition to such "model Tuning," one may legitimately "tune" to correct for under-resolution in engineering parametric studies, especially for trends (Oberkampf, 1998). The faintly pejorative association of model Tuning is deserved if every new data set requires re-tuning, but not so if reasonable universality is obtained. Bradshaw (1992) noted that "a simple model which has been carefully calibrated" [for a particular problem] "may out-perform more advanced models on its home ground. This may be called the First Law of Turbulence Modeling."

It is important to recognize that all of these activities (Verification of calculations, Calibration, Validation, and especially Certification) have associated with them error tolerances that cannot be arbitrarily defined universally but must be defined with reference to their intended uses (Marvin, 1988; Mehta, 1995; Melnik et al, 1996). Also, as noted above, Certification is a *programmatic* concept, rather than a scientific concept.