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SUCCESSIVE PROCEDURE FOR SOLUTION VERIFICATION BASED ON USER NEEDS

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ABSTRACT

This paper discusses a revised solution verification procedure for computational fluid dynamics simulations to estimate the uncertainties in the quantities of interest based on discretization error models. This proposed procedure builds upon current procedures described in ASME V&V 20 but provides more guidance in determining the necessary number of mesh levels to build reliable discretization error models. Such guidance is particularly useful for practicing engineers without prior experience in solution verification. The key features of this proposed solution verification procedure are the ability to determine the need for additional mesh levels iteratively and the seamless treatment for underdetermined, exact, and overdetermined solutions of the power series approximation to the discretization error models. This study applies the proposed procedure to a set of synthetic examples to demonstrate the revised procedure's clarity in determining the number of mesh solutions required for a reliable estimate of the discretization error in computational fluid dynamics settings. Additionally, this proposed procedure prevents a potential pathway in the current procedure in ASME V&V 20 that may lead to unreasonably small discretization errors.[1]

NOMENCLATURE

D Dimension of computational fluid dynamics problem
F_s Grid convergence index factor of safety
f Solution quantity of interest
f_∞ Extrapolated solution quantity of interest
h Mesh size parameter
N Number of cells or elements in a solution mesh
N_g Number of meshes solved for computational fluid dynamics problem
p Order of convergence
$\hat{p}$ Observed order of convergence
r Mesh refinement ratio
V_i Volume of cell or element i
α Power series coefficients

1 INTRODUCTION

This work proposes a revised procedure for conducting solution verification of computational fluid dynamics (CFD) simulations to estimate the uncertainties in quantities of interest (QOIs) based on discretization error models. Current procedures—notably, the *Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer* published by the American Society of Mechanical Engineers (i.e., ASME V&V

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20)—describe methods for known sets of meshes (i.e., grids) [1]. These procedures differ from standard analysis procedures used by practicing engineers, creating the potential for inappropriate application of the recommended methods.

It is common for many practicing engineers to first run a CFD simulation on a single initial mesh to check if the initial mesh is sufficient before conducting a mesh study with either successive refinement or coarsening. This approach is reasonable because meshing and computation take significant time and computational resources. Indeed, an engineer is unlikely to have a prescribed number of initial meshes prior to conducting a mesh study. With limited time and computational resources, engineers almost always aim to solve the minimum number of additional CFD solutions needed to estimate uncertainties in the QOIs. Therefore, there is a need for computational tools to evaluate whether the number of meshes they have currently solved is sufficient for the problem at hand.

ASME V&V 20 describes the procedure for solution verification in Section 2-4.1. This five-step procedure for uncertainty estimation defaults to using three mesh solutions for establishing an approximate error bound using the grid convergence index (GCI) method as a solution to a power series model of discretization error. In cases in which solution verification error and uncertainty terms are unacceptably large, more than three mesh solutions are required. The standard provides engineers two methods for improving estimates: using multiple sets of three mesh solutions or a least-squares solution to the power series. However, no further details on how to extend the study for an overdetermined solution are provided within the procedure itself.

For practicing engineers without prior experience in solution verification, how to deviate from the presented five-step procedure with more than three meshes may not be obvious. Furthermore, Section 2-5 of ASME V&V 20 (i.e., "Special Considerations") suggests a more encompassing approach in which the solution verification procedure of Section 2-4.1 involves only a single step. This section conceals the most important information because first-time readers will not likely understand this relationship. Because of this layout, this study posits that the ASME V&V 20 procedure for solution verification can be revised to better align with the expectations of practicing engineers looking for a method to reliably quantify the error in their CFD simulations.

The present work first describes the power–law model of discretization error along with how the model is solved for underdetermined, exact, and overdetermined solutions in Section 2. Then, this work briefly reviews the ASME procedure for solution verification in Section 3. Next, the present work describes the proposed procedure with subsections further elaborating each major step in Section 4. After presenting the procedure, its use is elucidated on a few synthetic example cases before discussing the difference in the present procedure from existing methods based on these examples; this comparison concludes the work (see Sections 5- 7).

2 POWER-LAW MODEL OF DISCRETIZATION ERROR

Power series expansion, such as the one shown in Eq. 1, is commonly used to describe discretization error of a numerical scheme (e.g., the finite-volume method or finite-element method).

$$f = f_\infty + \alpha_1 h + \alpha_2 h^2 + \alpha_3 h^3 + ..., \tag{1}$$

where f is the discrete solution QOI, f_∞ is the QOI with zero discretization error, h is a characteristic mesh size, and α_n are the series coefficients. The origin of the power series is the Taylor series expansion of the discrete solution about the exact solution [2]. The power series coefficients, α_n, contain the information from the unknown derivatives of the solution.

For a given solution, the power series can be simplified by considering the formal order of accuracy of the code. For example, a second-order code can be represented by the power series given in Eq. 2. The first-order error term is eliminated by the use of a second-order method; additionally, all higher-order error terms are combined.

$$f = f_\infty + \alpha_2 h^2 + O(h^3). \tag{2}$$

The power series can be further reduced to a single-term expansion by assuming the CFD solution is solved in the asymptotic regime where the error is dominated by the lowest-order error term, eliminating all higher-order errors. This reduction is shown in Eq. 3:

$$f \approx f_\infty + \alpha_2 h^2. \tag{3}$$

Richardson first used the power series to express discretization error in 1910 [3]; these methods are now called Richardson extrapolation methods because the power series model allows an engineer to extrapolate the known solution values to the zero-error limit by estimating f_∞. However, extrapolated values are not commonly reported even when the model is used for estimating discretization errors because of the limitations of the extrapolation model [2,4]. For more in-depth discussions on Richardson extrapolation, the authors recommend either the texts of Roache [5] or Oberkampf and Roy [2].

Generally, the realized order of convergence does not match the solver's formal order of accuracy. For example, problems with shocks will be at most first-order accurate at the shock with the first-order error term transported throughout the domain [2]. In general, a solution QOI will not converge at the formal order of accuracy because of artificial dissipation, solution singularities, switching functions, or other nonsmooth features of the problem that violate the simple power series model for discretization error. As such, the single-term power series for the solution is written with an unknown power, p, as in Eq. 4 [2]:

$$f = f_\infty + \alpha h^p. \tag{4}$$

Eq. 4 is a valid model for the discretization error when the model is solved in the asymptotic regime of the problem; it has three unknowns—f_∞, α, and p—and forms the basis for the most common forms of solution verification in CFD and this work. Next, this work discusses the various ways to solve Eq. 4 based on the number of CFD solutions an engineer has.

2.1 Solution with Known Convergence Order

For a small subset of problems, the realized convergence order of the solutions is known, permitting an *underdetermined* solution of the power series with only two mesh solutions by fixing the order of convergence. Although this method is not common because of the aforementioned issues, simply using three meshes is not computationally efficient when the order is known. Because the convergence order p is known, the following two-equation system can be used to solve for f_∞ and α:

$$\begin{aligned} f_1 &= f_\infty + \alpha h_1^p, \text{and} \\ f_2 &= f_\infty + \alpha h_2^p. \end{aligned}$$

In this equation, f_1 is the solution QOI to the fine mesh solution, and f_2 is the solution QOI to the coarse mesh solution. The two-equation system reduces to Eq. 5 [5]:

$$f_\infty = f_1 + \frac{f_1 - f_2}{r^p - 1}, \tag{5}$$

where $r = h_2/h_1$ is the mesh refinement ratio. The series coefficient is then solved using Eq. 6 [2]:

$$\alpha = \frac{f_1 - f_\infty}{h_1^p}. \tag{6}$$

2.2 Exact Solution to Power–Law Model

For the more common case in which the realized order of convergence is unknown, the exact solution to Eq. 4 can be found by solving the following three-equation system for f_∞, α, and p:

$$\begin{aligned} f_1 &= f_\infty + \alpha h_1^p, \\ f_2 &= f_\infty + \alpha h_2^p, \text{and} \\ f_3 &= f_\infty + \alpha h_3^p. \end{aligned}$$

For constant mesh refinement ratios, the observed order of convergence can be found using Eq. 7:

$$\hat{p} = \frac{\ln\left(\frac{f_3 - f_2}{f_2 - f_1}\right)}{\ln(r)}, \tag{7}$$

where $\hat{p}$ is the observed convergence order [2]. The extrapolated QOI and the series coefficient can then be computed using Eqs. 5 and 6, respectively.

For nonconstant refinement ratios, the transcendental equation in Eq. 8 must be solved:

$$\frac{f_3 - f_2}{r_{23}^{\hat{p}} - 1} = r_{12}^{\hat{p}} \left(\frac{f_2 - f_1}{r_{12}^{\hat{p}} - 1}\right). \tag{8}$$

This equation is most easily solved with an iterative direct substitution method. For specific schemes, see Refs. [1,2,5].

2.3 Overdetermined Solution to Power–Law Model

Finally, when more than three mesh solutions are considered, an overdetermined solution to Eq. 4 must be found. Considering more than three mesh solutions is helpful for many practical engineering problems because noise in the solutions can obscure the true solution to the power series. This work follows the ASME V&V 20 standard in recommending the use of the least-squares solution by Eça and Hoekstra [6]. The least-squares solution is found by minimizing Eq. 9. For recommended solution methods, see Refs. [1,2,5].

$$S(f_\infty, \alpha, \hat{p}) = \sqrt{\sum_{i=1}^{N_g} \left[f_i - \left(f_\infty + \alpha h_i^{\hat{p}}\right)\right]^2}. \tag{9}$$

3 EXISTING PROCEDURES

Arguably, the most important procedure for solution verification is the one detailed in Section 2-4 of ASME V&V 20 [1]. This procedure is functionally the same as the procedure presented in the 2008 announcement made by the *ASME Journal of Fluids Engineering* [7]. In essence, both sources detail a procedure to implement the GCI method [4], though some differences exist in the descriptive texts. Although individual articles or books may describe different solution procedures, the standard procedure described in ASME V&V 20 is important because it is generally the first reference used by practicing engineers before diving deeper into the literature. The standard procedure described in ASME V&V 20 consists of five steps. For ease of reading, this work lists the procedure here (with brief paraphrasing); for the full text, see ASME V&V 20 [1].

1. Define a representative mesh size h using the appropriate equation for the problem mesh (i.e., structured or unstructured).
2. Solve the problem on three significantly different meshes with recommendations that the grid refinement factor is greater than 1.3, refinement is systematic, and refinement is equal in all directions.
3. Solve for the observed order of convergence using the methods from Ref. [8]. Note that four meshes are required to demonstrate that the observed order of convergence is constant and that it may require more mesh solutions to demonstrate this property or provide a numerical uncertainty estimated less than other problem uncertainties.
4. Calculate the extrapolated QOI.
5. Calculate and report the QOI's relative error, estimated extrapolated relative error, and GCI. *Approximately one page of additional text follows this step with a detailed explanation about the appropriate use of GCI as an error measure that accounts for the uncertainties.*

This five-step procedure provides a simple approach for engineers to conduct solution verification for their CFD problems. To date, this five-step procedure has been effective in promoting solution verification and establishing it as an integral component of CFD analysis. However, it is the authors' opinion that this procedure can be improved.

First, this study proposes to recast the current procedure to iteratively determine the required number of mesh levels for building a reliable discretization error model. The current procedure can be read as a fixed procedure that heavily favors three-mesh solutions to the power–law model regardless if more mesh solutions are available. For some CFD problems, three-mesh solutions are simply not enough to build a reliable discretization error model due to noisy convergence of the solution QOIs. Section 2-5 of ASME V&V 20 recognizes this issue and suggests that engineers conduct an initial nominal solution on three to six meshes with different refinement levels. This suggestion aligns more closely with common practice but is not part of the explicit procedure. Furthermore, meshing and computations take significant time and computational resources, and without clear metrics on when more than three-mesh solutions are needed, engineers will most likely default to using three-mesh solutions and call it "good enough." Determining the number of required mesh levels a priori is also challenging because it largely depends on the CFD problem at hand. Thus, an iterative procedure will be more robust and efficient. The improved robustness comes from clear metrics for determining the minimum number of mesh levels required to build a reliable discretization error model for the CFD problem at hand. This work notes that without a reliable discretization error model, accurate estimates of uncertainties in the QOIs cannot be obtained. The improved efficiency comes from the fact that engineers do not need to waste their time and computational resources to generate a large (fixed) number of meshes a priori but rather need to spend their time and resources efficiently by generating one additional mesh at a time as needed throughout the iterative procedure.

Second, this work provides clear metrics to determine if the discretization error model is reliable. The current procedure heavily favors three-mesh solutions without clear metrics for assessing the reliability of the resulting discretization error model. Even more vexing is that the current procedure accepts the resulting discretization error of a three mesh study if the solution verification error and uncertainty terms are small compared to other error and uncertainty terms. This metric is vulnerable to accepting unreasonably optimistic discretization error estimates if the three-mesh solution returns a convergence order greater than the code's theoretical order of convergence. The metrics proposed in this work will evaluate the uncertainty of the discretization error model independently of other error terms and will guide the iterative procedure in determining the minimum number of mesh levels required to build a reliable discretization error model for the CFD problem at hand.

3.1 A Least-Squares Solution Procedure

Of all other procedures, this work highlights the one described by Eça and Hoekstra in 2014 [9]. Their least-squares solution for the GCI is in the nonmandatory appendices of the ASME V&V 20 standard [1]; however, V&V 20 only includes the least-squares solution and not the full procedure described later in 2014. This procedure requires a minimum of four mesh solutions because the least-squares solution requires an overdetermined system. Also, this procedure is not iterative; engineers must deduce on their own if their analysis should be rerun with additional mesh solutions. Notably, though, the method evaluates the quality of the discretization error model. The following is an abbreviated summary of Eça and Hoekstra's procedure [9] which assumes the code's formal order of accuracy is two.

1. First, the power series approximation of the discretization error model is fitted in both a weighted and nonweighted approach.
   (a) If the computed order of convergence is between 0.5 and 2, the fit is deemed valid.
   (b) If the computed order of convergence is above 2, the lowest standard deviation fit between a first-order and second-order power series is taken.
   (c) If the computed order of convergence is below 0.5, the lowest standard deviation fit between a first-order, second-order, and mixed first- and second-order power series is taken.
2. Determine the range of data parameters.
3. Assign a factor of safety of 1.25 if the computed order of convergence is between 0.5 and 2.1 and the standard devia-

tion of the fit is less than the data range. Otherwise, assign a value of 3.
4. Compute the uncertainty of the QOI.

Eça and Hoekstra's procedure evaluates the quality of the power series fit of the discretization error model, and it has served the community well. However, Eça and Hoekstra's procedure still lacks guidance in determining the required number of mesh levels to build a reliable discretization error model for the problem at hand; it simply trusts the engineers to know how many more mesh solutions are needed beyond the required four mesh solutions. As such, their procedure is not iterative. Per previous discussions, this work deems these noniterative procedures as inaccessible to engineers unfamiliar with solution verification. For this reason, the authors believe the conjecture from the introduction stands in that the ASME V&V 20 solution verification procedure can be improved to better support engineers.

4 PROPOSED PROCEDURE

This work combines existing solution verification procedures [1, 9] and creates a complete procedure that can handle underdetermined, exact, and overdetermined solutions to the power–law model of discretization error. To address the question of how many mesh levels are needed to build a reliable error model, this work formulates an iterative procedure that adds one mesh level at a time as needed. Notably, the necessary number of mesh levels is unlikely to be known beforehand. The revised procedure is described in the following list; all clarifying texts are in the subsections for these steps.

1. Obtain an initial solution to the CFD problem on a mesh constructed based on the expert judgment of the engineer.
2. Identify the characteristic mesh size of the problem.
3. Create a refined or coarsened mesh as part of a valid mesh sequence.
4. For problems with a known convergence order, solve the power–law model for f_∞ and h with the two QOI values. Proceed to Step 8. Note that it is uncommon to know the convergence order.
5. For problems with an unknown convergence order, solve the power–law model for f_∞, h, and p with the three QOI values. Proceed to Step 7.
6. Solve the overdetermined solution to the power–law model for f_∞, h, and p with the QOI values from the N_g mesh solutions.
7. Evaluate the accuracy of the power–law model based on recommended criterion in explanatory text and problem needs. If sufficient, proceed to Step 8. Otherwise, repeat Step 3, then proceed to Step 6.
8. Report the uncertainty measure of your choice for the QOI value (on the nominal solution mesh), the observed order of convergence, and sufficient details on the solution verification process to repeat the procedure.

The solution verification procedure presented here primarily differs from the existing procedure described in the ASME V&V 20 standard by iteratively determining if additional mesh solutions are needed to construct a reliable discretization error model. The iterative nature of this proposed procedure helps engineers use their limited time and computational resources efficiently because they now only need to generate the minimum number of meshes required for a given problem. Additionally, the proposed procedure includes an explicit step to evaluate the accuracy of the power–law model. In summary, this proposed procedure more clearly elucidates the end goal and requirements of solution verification for engineers who use the ASME V&V 20 standard to guide their analyses.

4.1 Explanation of Step 1

The solution verification procedure demands a well-defined CFD problem and a well-resolved base solution. The result of a solution verification procedure is also only valid for a given set of CFD parameters and a given sequence of meshes; any changes in parameters or meshes will require rerunning of the solution verification procedure. It is also crucial that the CFD problem is solved on a sequence of meshes. As such, it would be unwise for engineers to create a sequence of meshes before determining the validity of the initial mesh for the CFD problem (i.e., before obtaining a well-resolved base solution); the initial mesh dictates the additional meshes required to form a sequence. To form a sequence of meshes, engineers may choose to create a finer or coarser mesh compared with the initial mesh. For example, engineers may choose to create a coarser mesh for a detailed nominal study or a finer mesh for a CFD problem setup for a parameter study. This step aligns with the suggestion in Section 2-5 of ASME V&V 20.

4.2 Explanation of Step 2

For general CFD problems on unstructured meshes, the characteristic mesh size can be computed using Eq. 10:

$$h = \left[\frac{\sum_{i=1}^{N} V_i}{N}\right]^{1/D}, \tag{10}$$

where N is the number of cells or elements in the domain, V_i is the volume of the ith cell or element, and D is the dimension of the mesh [8]. Notably, Eq. 10 is not valid for all meshes—most notably not for meshes with nonuniform refinement or inconsistent refinement [2]. The engineer must determine that the analyzed meshes are well-described by the characteristic size and comprise a mesh refinement sequence [10]. This step is qualitatively similar to Step 1 in the ASME V&V 20 standard [1]. However, this work emphasizes that a well-resolved base solution must be found before a characteristic size for the problem is specified.

4.3 Explanation of Step 3

Solution verification is agnostic as to whether a sequence of meshes is generated by refining or coarsening the initial mesh as long as the meshes remain valid for the CFD problem. When the CFD problem is computationally tractable on refined meshes, this work prefers that the sequence is constructed based on these refined meshes because they will produce smaller discretization errors; however, coarsened meshes can be used effectively if the CFD solution still lies in the asymptotic regime. A refinement ratio, $r = h_{\text{coarse}}/h_{\text{fine}}$, greater than 1.3 is recommended as a best practice to generate a sufficient difference between the solution QOIs to mask solution noise [1, 7]. Meshes with differences as small as a single cell or element are valid, though an unreasonable number of mesh solutions will typically be required to obtain an accurate fit to the power–law model of discretization error [5]. Additionally, refinement should be global and as uniform as possible. Nonuniform refinement can return erroneous orders of convergence [11] and is best handled by independent grid refinement studies [4].

4.4 Explanation of Step 4

Step 4 is used for problems in which the convergence order of the problem is known. To claim that the convergence order is known, engineers must first justify that their problem meets this condition. One way is by demonstrating that a previous calculation on a sufficiently similar problem established the convergence order of the problem and does not contain a condition that may change this convergence order for the differences in the problems. More importantly, code verification demonstrating the formal order of a solver for separate verification problems does not meet this standard. This work does not try to establish the necessary limits for this condition.

4.5 Explanation of Step 5

The next step is to obtain three-mesh solutions and construct the power–law model of discretization error. For most analyses, this step will be the first discretization error computation. Engineers may use their preferred solution strategy to solve the three-equation system. In ASME V&V 20, the three listed equations to solve the system (2-4-5, 2-4-6, and 2-4-7) are easy to implement [1], though they do not include an explicit iterative index to clearly denote that a fixed point iteration is required, as shown in Eq. 8.74 from Oberkampf and Roy [2].

4.6 Explanation of Step 6

To solve the overdetermined power–law model, this work recommends the least-squares solution of Eça and Hoekstra [6], as discussed previously. In 2014, Eça and Hoekstra created a full solution procedure, which solves both the unweighted and weighted models [9]. Although these models are valuable, the solution verification community has not yet determined their preferred approach. This study has no preference at this time, though it uses the unweighted method in the example problem. Also, notably, engineers may use other methods to solve the overdetermined power–law model.

The proposed procedure does not yet handle fitting a mixed-order, power–law model, as in the 2014 procedure [9]. Such methods will be useful for CFD problems with non-monotonic convergence [12], which is commonly observed in many practical CFD problems. The additional methods needed to handle non-monotonic convergence are left for future work. Some questions to be answered include whether these methods should (1) use arbitrary orders or include a first-order term explicitly and (2) capture the oscillatory convergence.

4.7 Explanation of Step 7

The accuracy of the power–law model can be evaluated in multiple ways. Regardless of the chosen methodology, it is important to first determine if the computed order of convergence is valid. The generally accepted bounds are 0.5 and 2 [2, 5, 9], though new high-order codes will extend this upper order to the formal order of the solver. As a starting point, this procedure recommends that the valid range for an observed order of convergence is between 0.5 and the formal order of the solver; a 5% buffer is allowed over the formal order of convergence to account for small numerical errors, though the solution should use the formal order when the observed order is in this margin. These bounds align with the work of Eça and Hoekstra [9].

The criterion discussed in the previous paragraph is insufficient to convincingly establish the reliability of the power–law model alone, though it is a good start. The authors do not have sufficient experience with other methods to advocate for them here. However, it will be important to establish these methods for the standard so there is more than a single criterion on the observed order for the modeling effort.

One common approach is to model subsets of the data and confirm that each submodel's observed order agrees. For example, three overlapping three-mesh solutions would be solved over a total of five meshes. If the observed order for all three solutions was within 5%, engineers would trust the model. However, such a solution strategy contradicts the goal of an iterative method designed to evaluate on the fewest number of meshes possible. Modeling subsets of data is appealing but will quickly become expensive for general applications, though it may be recommended for critical applications.

4.8 Explanation of Step 8

The reported error and uncertainty measurements are a function of both the method used and the desired measurement type. For example, error estimates may be normalized or not, include a factory of safety, encompass a different confidence interval, or assume an underlying error distribution [1]. This work recommends the GCI method for reporting error estimates because it is a well-established and well-accepted method [1]. Specifically, the non-normalized GCI computation given in Eq. 11 is recommended for fine mesh solutions [2] and Eq. 12 for coarser meshes [2]. In both equations, F_s is a factor of safety used to approximate a 95% confidence interval based on the expert judgment of Patrick Roache [4,5].

$$\mathrm{GCI}_{\mathrm{fine}} = \frac{F_s}{r^{\hat{p}} - 1}|f_2 - f_1|. \tag{11}$$

$$\mathrm{GCI}_{\mathrm{coarse}} = r^{\hat{p}}\mathrm{GCI}_{\mathrm{fine}}. \tag{12}$$

For a community standard, it would be beneficial to detail alternative reporting options like ASME V&V 20 currently does. For example, ASME V&V 20 provides a conversion of the GCI metric, which is based on an ad-hoc 95% confidence interval, to an uncertainty interval based on one standard deviation to align with new international standards [1]. Long-term developments to remove the ad hoc nature of the GCI method will also be desirable, such as the discontinuous nature of only using factors of safety of 1.25 and 3. Smoother behavior, like that shown in the factor of safety method of Xing and Stern [13], is a more natural fit to an iterative procedure such as the one detailed in this work.

5 EXAMPLES

This section demonstrates the application of the proposed iterative procedure to a synthetic CFD analysis that is representative of the analysis a practicing engineer may need to do. This synthetic example will assume that the engineer is using a second-order, finite-volume CFD solver and is tasked with evaluating the pressure drop across the valve of a new system based on varying multiple input parameters to find the best design. As such, the engineer conducts the solution verification process to establish the uncertainty of the pressure drop in the coarse mesh solution for parametric studies.

First, the case when the analysis has a valid three-mesh solution is considered. Next, the problem is evaluated when it requires an overdetermined solution to the power–law model (i.e., four or more mesh solutions are considered). The synthetic example used in this work is based on the authors' experience running real analyses and is utilized to highlight the revised procedure without requiring the complicated details of multiple CFD analyses. To highlight the discretization error in this example, the engineer is assumed to solve each mesh to machine precision, so the iterative error is zero and all numerical uncertainty is captured by the discretization error estimated by the power–law model.

5.1 Three-Solution Problem

The simplest solution verification process involves three-mesh solutions. The engineer starts the solution verification procedure (i.e., Step 1) by obtaining a nominal solution to their CFD problem. The next step (i.e., Step 2) requires them to compute the characteristic mesh size. For this example, consider a 1 m^3 domain with 1,000,000 cells. Using Eq. 10, the characteristic length for this first mesh is $h_1 = 10$ mm. Proceeding to Step 3, the engineer creates another mesh. In this example, assume that the engineer uses the nominal simulation for parametric studies. Thus, they create refined meshes for the solution verification process; this practice aligns with the recommendation that refined meshes are preferred when computationally affordable to ensure asymptotic behavior. The engineer applies a refinement factor of 1.3, resulting in a mesh with 2,197,000 cells and a characteristic length of $h_2 = 7.69$ mm. Because the convergence order for the problem is unknown, the engineer repeats Step 3 to create a third mesh with 4,826,809 cells and a characteristic length of $h_3 = 5.92$ mm.

Next, the engineer evaluates the solution discretization error in Step 5. Because the refinement ratio is constant, they solve for p using Eq. 7. For this synthetic example, the engineer aims to estimate the pressure loss through a to-be-installed valve for their system. The estimated pressure losses for the three-mesh solutions are $f_1 = 10$, $f_2 = 12$, and $f_3 = 13.2$ kPa. The resulting observed order of convergence is 1.95 with $f_\infty = 15$. Based on the order limits from Step 7, the engineer assesses the power–law model and finds it to be sufficiently accurate. Therefore, they proceed to Step 8.

In Step 8, the engineer chooses to use the GCI method to report their estimated numerical uncertainty. First, they compute the fine mesh GCI using Eq. 11 and obtain $\mathrm{GCI}_{\mathrm{fine}} = 2.25$. Second, they compute the coarse mesh GCI using Eq. 12 with $\mathrm{GCI}_{\mathrm{coarse}} = 6.25$. The overall refinement factor is $r = 1.69$. Finally, they report the observed order of convergence, the nominal mesh GCI value, and the minimum information needed to recreate the study for Step 8; these values are shown in Table 1. Additionally, Figure 1 plots the data, f_∞, and the fit to the power–law model. For this problem, $\mathrm{GCI}_{\mathrm{coarse}}$ is large enough that a reasonable engineer would likely not proceed with the parametric study using the coarse mesh as the numerical uncertainty interval exceeds 50% of the coarse mesh's estimated pressure drop. Instead, they would use the finer mesh and adjust their parametric study based on the computational resources available.

TABLE 1. REPORTED VALUES FOR THREE-SOLUTION PROBLEM

Parameter	Value	Unit
h_1	10	mm
h_2	7.69	mm
h_3	5.92	mm
f_1	10	kPa
f_2	12	kPa
f_3	13.2	kPa
$\hat{p}$	1.95	
f_∞	15	kPa
GCI_1	6.25	kPa

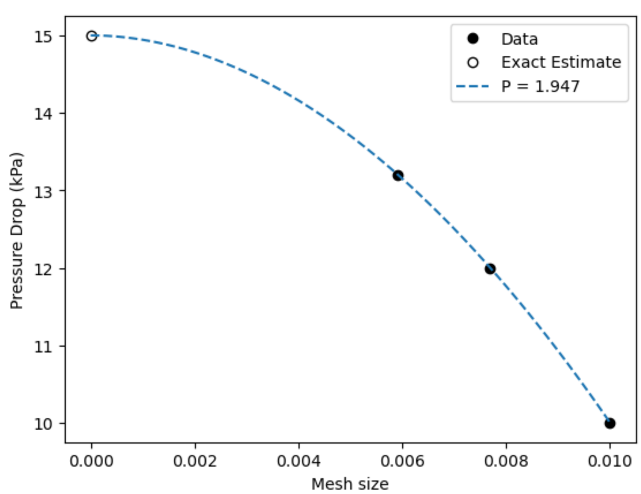

FIGURE 1. PLOT OF THE POWER–LAW MODEL FOR THREE-SOLUTION PROBLEM

5.2 Overdetermined Solution Problem

Next, this study considers an example where more than three mesh solutions are needed to establish a reliable error model. If the three mesh values in the prior analysis were instead $f_1 = 10$, $f_2 = 12.2$, and $f_3 = 13.2$, the observed convergence order computed in Step 5 will be $\hat{p} = 3$. Note this occurs simply by changing the value of f_2 from 12 to 12.2. Therefore, Step 7 of the procedure reveals that a fourth mesh is needed because the power–law model of discretization error is insufficiently reliable based on the fact that the observed order of accuracy is higher

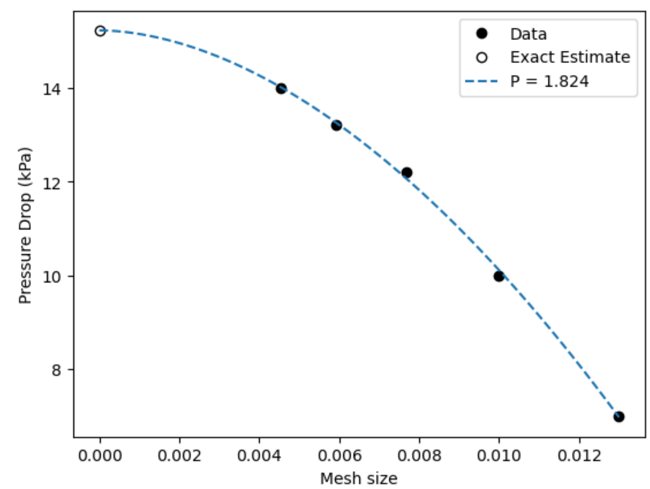

FIGURE 2. PLOT OF POWER–LAW MODEL FOR OVERDETERMINED SOLUTION PROBLEM

than the formal order of the CFD solver (which is assumed to be a second-order, finite-volume code). Repeating Step 3, the engineer creates an additional mesh with a 1.3 refinement factor, resulting in a mesh with a total mesh count of 10,604,500 cells and a characteristic size of $h_4 = 4.55$ mm. For this mesh, $f_4 = 14$ kPa.

Proceeding to Step 6, the engineer solves the overdetermined power–law model using the least-squares solution shown in Eq. 9. The solution returns $\hat{p} = 2.25$, which again fails the sufficiency criteria of Step 7. Therefore, the engineer repeats Step 3. This time, the increasing mesh requirements will make a refined mesh too expensive for the analysis, so the engineer coarsens the nominal mesh by a factor of 1.3 to create a mesh with 455,166 cells and a characteristic length of $h_5 = 13$ mm. For this mesh, $f_5 = 7$ kPa.

Finally, the overdetermined solution to the power–law model returns an observed convergence order of $\hat{p} = 1.82$, which passes the checks in Step 7 of the procedure. As in the previous example, the engineers choose to report the numerical uncertainty using the GCI metric. Table 2 and Figure 2 show the result of this solution verification. The GCI for the overdetermined solution is slightly higher than for the three-mesh solution in the previous example mainly because of the slightly lower (observed) order of convergence. Notably, the nonexact interpolation of the least-squares solution to the power–law model is not reflected in the final uncertainty estimate. Again, the engineer would use these numerical uncertainty estimates to determine the correct mesh to use for their parametric study.

TABLE 2. REPORTED VALUES FOR OVERDETERMINED SOLUTION PROBLEM

Parameter	Value	Unit
h_1	10	mm
h_2	7.69	mm
h_3	5.92	mm
h_4	4.55	mm
h_5	13	mm
f_1	10	kPa
f_2	12	kPa
f_3	13.2	kPa
f_4	14	kPa
f_5	7	kPa
$\hat{p}$	1.82	
f_∞	15.22	kPa
GCI_1	6.85	kPa

6 DISCUSSION

The example problems presented in this study show the utility of this iterative solution verification procedure on CFD problems. Engineers can follow the same procedure while transitioning from an exact to an overdetermined solution to the power–law model, eliminating potential error points in the process and potentially reducing the number of meshes that need to be generated. Additionally, Step 7 ensures the engineers evaluate the accuracy of the power–law model in addition to the problem's numerical uncertainty. Also, the difference between the presented procedure and the ASME V&V 20 procedure was noted for the example presented in Section 5.2 (i.e., the example with $f_1 = 10$, $f_2 = 12.2$, and $f_3 = 13.2$). At this point, the exact solution to the power–law model has an observed convergence order of 3. Engineers following ASME V&V 20 will compute the error and uncertainty terms for this solution. For $\hat{p} = 3$, GCI_1 is 5.04. Based on the guidance in Step 3 of ASME V&V 20's procedure, engineers may proceed if the error term is smaller than others in their analyses [1]. However, in this case, engineers would be inadvertently accepting an invalid solution to the power–law model, which shows the solution converging more rapidly than possible for a second-order accurate CFD solver. The presented procedure prevents this possibility by requiring engineers to evaluate the accuracy of the power–law model in Step 7.

7 CONCLUSION

This work presents a revised solution verification procedure for CFD problems to provide accurate estimates of the uncertainties in the QOIs. This procedure is more accessible to practicing engineers, especially those without prior experience in solution verification. The approach was to recast the procedure presented in ASME V&V 20 as an iterative procedure and add a step to evaluate the reliability of the discretization error model. The iterative procedure guides engineers in determining the minimum number of mesh levels required to construct a reliable discretization error model. A set of synthetic examples demonstrates the ease of following the revised procedure and highlights a case where this procedure prevents engineers from inadvertently accepting an incorrectly small uncertainty estimate for their QOI if they were to follow the ASME V&V 20 procedure.

For future work, this iterative procedure will benefit from more detailed descriptions of how engineers can construct and evaluate meshes to ensure a valid mesh sequence is used in their analysis. The procedure will also benefit from more rigorous testing to ensure that it will not permit invalid solutions to the power–law model. Additional future work includes further criteria to evaluate the acceptableness of the power–law model, the ability to fit non-monotonic data with a multiterm power series, tools to handle non-convergence, and criteria for excluding solutions not in the asymptotic regime.

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