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ON THE APPLICATION OF THE AREA METRIC TO VALIDATION EXERCISES OF
STOCHASTIC SIMULATIONS

L. Eça

MARIN Academy, IST ULisbon
Email: luis.eca@ist.utl.pt

K. Dowding

Sandia National Laboratories
Email: kjdowdi@sandia.gov

P.J. Roache

Consultant
Email: hermosa@sdcc.org

ABSTRACT

This paper discusses the application of the Area Metric to the quantification of modeling errors. The focus of the discussion is the effect of the shape of the two distributions on the result produced by the Area Metric. Two different examples that assume negligible experimental and numerical errors are presented: the first case has experimental and simulated quantities of interest defined by normal distributions that require the definition of a mean value and a standard deviation; the second example is taken from the V&V10.1 ASME Standard that applies the Area Metric to quantify the modeling error of the tip deflection of a loaded hollow tapered cantilever beam simulated with the static Bernoulli-Euler beam theory.

The first example, shows that relatively small differences between the mean values are sufficient to filter the information contained in the standard deviation. Furthermore, the example of the V&V10.1 ASME Standard produces an Area Metric equal to the difference between the mean values of experiments and simulations. Therefore, the error quantification is reduced to a single number that is obtained from a simple difference of two mean values. This means that the Area Metric fails to reflect a dependence for the difference in the shape of the distributions representing variability.

The paper also presents an alternative version of the Area Metric that does not filter the effect of the shape of the distributions by utilizing a reference simulation that has the same mean value of the experiments. This means that the quantification of the modeling error will have contributions from the difference in mean values and from the shape of the distributions.

1 INTRODUCTION

The assessment of the quality of computational simulations requires the quantification of the modeling error resulting from the assumptions and approximations included in the mathematical model that represents the physical reality.

Nowadays, it is commonly accepted [1–4] that the goal of validation is exactly this quantification of the modeling error, which is performed by comparing numerical results with experimental data for a given quantity of interest (also known as validation variable, system response or figure of merit).

The quantification of modeling errors for a given quantity of interest is not as trivial as the highly popular graphical comparisons of numerical and experimental results might suggest. Experimental measurements are affected by measurement uncertainties and variability in material properties, heat transfer coefficients and/or boundary conditions, [5]. Simulations include numerical uncertainties and input parameters uncertainties, which are related to the material properties, heat transfer coefficients and/or boundary conditions.

Deterministic simulations use nominal values of the input parameters (scalar quantities) to perform simulations. On the other hand, stochastic approaches characterize the uncertain input parameters with probabilistic distributions. These distributions must be propagated through the mathematical/computational model to obtain the quantities of interest, which will also be represented by a probabilistic distribution. The quantification of modeling errors in stochastic simulations is based on the comparison of probabilistic distributions obtained from experiments and simulations.

The experimental characterization of the quantity of interest can be affected by measurement uncertainty and statistical con-

vergence (number of samples available), whereas the simulations results for the quantity of interest can be affected by numerical uncertainty (discretization, iterative and round-off errors), uncertainties in the definition of the input parameters distributions and statistical convergence. Therefore, multiple probabilistic distributions (probabilistic boxes) [6] may be required. However, in the present study, following [7] we focus on problems where experimental measurement uncertainty, numerical uncertainty and uncertainties in the input parameters distributions are negligible. In these conditions, the probabilistic distributions that characterize the quantity of interest are only a consequence of variability in material properties, any other problem parameters and/or boundary conditions. Furthermore, statistical convergence is assumed to be achieved in experiments and simulations.

The selected conditions are ideal for the application of the Area Metric presented in [7], which is a Validation metric that quantifies the modeling error when the experimental and simulations results have statistically converged, i.e. when the number of samples in experiments and simulations is sufficiently large. In the Area Metric, the challenging task of obtaining a single number from the differences between two distributions is accomplished using the absolute differences between cumulative distribution functions (CDF).

As stated in [7], if the two CDF's exhibit negligible intersection the Area Metric is equal to the difference between the mean values of the two distributions and so it filters the information contained in the type of distributions that represent the experiments and simulations. This would be a welcomed result if the Area Metric became insensitive to the type of distributions only for large differences between the mean values. However, the exercise reported in [8] for the V&V10.1 example [9] showed that small differences in the mean values (8.4% of the mean experimental value) are sufficient to obtain a negligible influence of the shape of the distributions. Therefore, the objectives of the present paper are:

1. Quantify the difference between the mean values of the experimental and simulations CDF's that leads to a negligible influence of the shape of the distributions;
2. Suggest a modification to the Area Metric as presented in [7] that does not ignore the discrepancies in shape of the experimental and simulations distributions for problems with negligible intersection of the CDFs.

The first objective is accomplished using normal distributions¹ defined by mean values and standard deviations of experiments and simulations. In this case, it is possible to quantify the Area Metric as a function of the mean values and standard deviations of the two distributions and quantify the difference in mean values that leads to a negligible contribution of the standard deviations (shape of the distributions).

The exercise performed with the normal distributions suggested an alternative formulation of the Area Metric. The proposed formulation keeps the contribution of the different shapes of the experimental and simulations distributions independently of the difference between mean values.

The remainder of this paper is organized as follows: section 2 describes the Area Metric and the alternative formulation proposed in this study; the outcome of the area metric as a function of the mean values and standard deviations of normal distributions that characterize the experimental and simulation data is presented and discussed in section 3 and section 4 presents the results of the two formulations of the Area Metric for the example presented in V&V10.1; Conclusions of this study are summarized in section 5.

2 AREA METRIC

For a given Quantity Of Interest ϕ defined by an experimental probability density function ($PDF_D(\phi)$) and a simulations $PDF_S(\phi)$, the area metric requires the calculation of the cumulative distribution functions $CDF_X(\phi)$

$$CDF_X(\phi) = \int_{-\infty}^{\phi} PDF_X(\phi) d\phi, \quad (1)$$

where X is D for the experiments and S for the simulations, respectively.

As presented in [7], the Area Metric $M(\phi)$ is defined by

$$M(\phi) = \int_{-\infty}^{+\infty} |CDF_S(\phi) - CDF_D(\phi)| d\phi. \quad (2)$$

In [9], the value of area metric is made dimensionless using the mean value $\mu_D(\phi)$ of the experimental $PDF_D(\phi)$.

Figure 1 illustrates the determination of the Area Metric for two cases where the quantity of interest ϕ of experiments and simulations is defined by normal distributions. The figure presents a case with a difference between the mean values $\Delta\mu = \mu_S - \mu_D = 0.2\mu_D$ (top plots) and another with $\Delta\mu = \mu_S - \mu_D = \mu_D$ (bottom plots). $M(\phi)$ corresponds to the gray area of the right plots. For $\Delta\mu = 0.2\mu_D$, there is intersection of the two CDF's and so the differences in standard deviations σ_S and σ_D will contribute to $M(\phi)$. On the other hand, with $\Delta\mu = \mu_D$ there is a negligible area of intersection and so $M(\phi)$ will be almost identical to $|\mu_S - \mu_D|$.

2.1 Proposal of an Alternative Area Metric

In a stochastic simulation, it is not expected that the modeling error is independent of the shape distribution, which is the result obtained from the Area Metric when there is a negligible

¹Other types of distributions could be used to make an equivalent exercise.

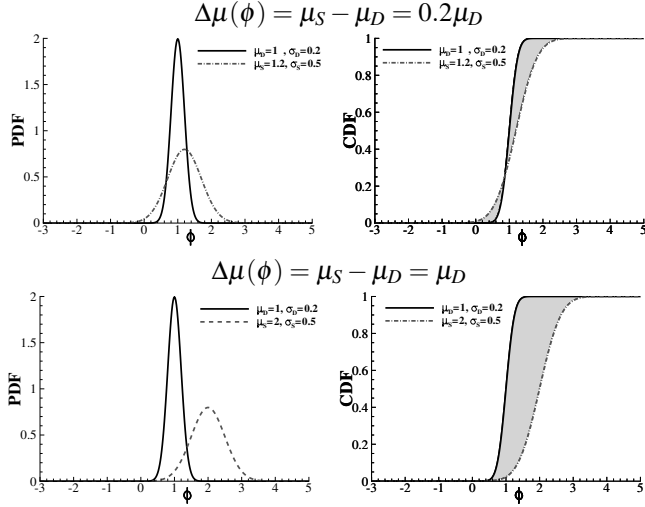


FIGURE 1. Illustration of the determination of the Area Metric (gray area in the right plots) for two cases with quantities of interest defined by normal distributions.

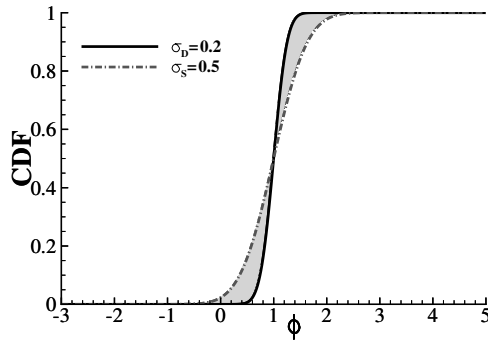


FIGURE 2. Illustration of the determination of the contribution of the shape of the distributions for the alternative Area Metric (gray area in the right plots) proposed in this work.

area of intersection between the two CDF's. Therefore, we propose an alternative formulation of the Area Metric that does not filter the information of the shapes of the distributions for any value of $\Delta\mu$.

The alternative version of the Area Metric is defined by

$$M_a(\phi) = |\mu_S(\phi) - \mu_D(\phi)| + M_o(\phi), \quad (3)$$

where

$$M_o(\phi) = \int_{-\infty}^{+\infty} |\text{CDF}_S(\phi^*) - \text{CDF}_D(\phi)| d\phi, \quad (4)$$

and²

$$\phi^* = \phi - (\mu_S(\phi) - \mu_D(\phi)). \quad (5)$$

This guarantees that $\mu_S(\phi^*) = \mu_D(\phi)$ and $\sigma_S(\phi^*) = \sigma_S(\phi)$ and so $\Delta\mu$ is removed from the integral of the differences between the two CDF's included in equation (5). For the two cases, illustrated in figure 1, the $\text{CDF}_S(\phi^*)$ are identical and the contribution of the shape of the distributions ($M_o(\phi)$) to $M_a(\phi)$ is illustrated in figure 2. The same area is valid for the two cases presented in figure 1, but $M_a(\phi)$ will not be identical because the difference between mean values ($\mu_S - \mu_D$) is not identical in both cases. Note that the areas illustrated in figure 1 correspond to $M(\phi)$, whereas the area represented in figure 2 corresponds only to the contribution of the different shapes of the distributions ($M_o(\phi)$).

3 AREA METRIC FOR QUANTITIES OF INTEREST DEFINED BY NORMAL DISTRIBUTIONS

The goal of this study is to quantify the contribution of the shape of the experimental and simulations distributions to $M(\phi)$ as a function of the difference between the mean value of the $\text{PDF}_S(\phi)$ and $\text{PDF}_D(\phi)$, $\mu_S(\phi)$ and $\mu_D(\phi)$, respectively.

The definition of the area metric $M(\phi)$, equation (2), does not impose any restriction to the type of distribution that leads to the experimental and simulations CDF's. In fact, these functions can be determined from a discrete set of samples, as illustrated in [9]. However, in order to assess the effect of the variability in the experimental and simulations data it is convenient to use CDF's that allow the analytic determination of $M(\phi)$. Several options could be used to achieve such result, as for example uniform, triangular or normal distributions. In the present study, we have used normal distributions. However, equivalent results can be obtained for the uniform and triangular distributions.

3.1 Probability density function, PDF

For a variable ϕ , a normal PDF is defined by

$$\text{PDF}(\phi) = \frac{1}{\sigma(\phi)\sqrt{2\pi}} e^{-\frac{1}{2} \left(\frac{\phi - \mu(\phi)}{\sigma(\phi)} \right)^2}, \quad (6)$$

where $\mu(\phi)$ is the mean value of the distribution and $\sigma(\phi)$ is the standard deviation

² ϕ^* can be interpreted as the result of a calibrated model.

3.2 Cumulative distribution function, CDF

The cumulative distribution function CDF defined by equation (1) is obtained from

$$\text{CDF}(\phi) = \frac{1}{2} \left[1 + \text{erf} \left(\frac{\phi - \mu_\phi}{\sigma_\phi \sqrt{2}} \right) \right], \quad (7)$$

where erf stands for the error function.

3.3 Area Metric, $M(\phi)$

Substituting the analytic definition of the CDF for a normal distribution in equation (2) we obtain:

$$M(\phi) = \frac{1}{2} \int_{-\infty}^{+\infty} \left| \text{erf} \left(\frac{\phi - \mu_S(\phi)}{\sigma_S(\phi) \sqrt{2}} \right) - \left(\frac{\phi - \mu_D(\phi)}{\sigma_D(\phi) \sqrt{2}} \right) \right| d\phi. \quad (8)$$

The value of $M(\phi)$ depends on the point where the simulations CDF_S(ϕ) and experimental CDF_D(ϕ) intersect, ϕ_I , which can be determined analytically.

$$\frac{\phi_I}{\mu_D(\phi)} = \frac{\left(\frac{\sigma_S(\phi)}{\sigma_D(\phi)} - \frac{\mu_S(\phi)}{\mu_D(\phi)} \right)}{\left(\frac{\sigma_S(\phi)}{\sigma_D(\phi)} - 1 \right)}. \quad (9)$$

Equation (9) shows that there is no intersection between the two CDF's when $\sigma_{S_\phi} = \sigma_{D_\phi}$, which leads to $M(\phi) = |\mu_S(\phi) - \mu_D(\phi)|$. Therefore, when the variability in the experiments and simulations is identical, the area metric does not include any contribution of $\sigma_D(\phi)$ and $\sigma_S(\phi)$, which is the expected result.

The advantage of using normal distributions for the experimental and simulation data is that $M(\phi)$ can also be calculated analytically when $\sigma_D(\phi) \neq \sigma_S(\phi)$.

$$\frac{M(\phi)}{|\mu_D(\phi)|} = (M_\mu(\phi) + M_\sigma(\phi)), \quad (10)$$

where

$$M_\mu(\phi) = \left| \text{erf} \left(\frac{\frac{\phi_I}{\mu_D(\phi)} - 1}{\frac{\sigma_D(\phi)}{\mu_D(\phi)} \sqrt{2}} \right) \left(1 - \frac{\mu_S(\phi)}{\mu_D(\phi)} \right) \right| \quad (11)$$

and

$$M_\sigma(\phi) = \left| \frac{\sigma_D(\phi)}{\mu_D(\phi)} \sqrt{\frac{2}{\pi}} \left(1 - \frac{\sigma_S(\phi)}{\sigma_D(\phi)} \right) \right| e^{-\left(\frac{\frac{\phi_I}{\mu_D(\phi)} - 1}{\frac{\sigma_D(\phi)}{\mu_D(\phi)} \sqrt{2}} \right)^2}. \quad (12)$$

Equations (10) to (12) show that $M(\phi)/|\mu_D(\phi)|$ depends only on three ratios:

1. Standard deviation of the experimental distribution over the mean value of the experiments, $\sigma_D(\phi)/\mu_D(\phi)$;
2. Mean value of the simulations distribution over the mean value of the experiments, $\mu_S(\phi)/\mu_D(\phi)$;
3. Standard deviation of the simulations distribution over the standard deviation of the experiments, $\sigma_S(\phi)/\sigma_D(\phi)$.

The contribution of the variability of the experimental and simulation distributions to the value of the area metric can be obtained from

$$\frac{\Delta M(\phi)}{M(\phi)} = 1 - \frac{|\mu_S(\phi) - \mu_D(\phi)|}{M(\phi)}. \quad (13)$$

Equation (13) quantifies the contribution of the differences between the shapes of the CDF_S and CDF_D to $M(\phi)$ as a function of $\mu_S(\phi)/\mu_D(\phi)$, $\sigma_D(\phi)/\mu_D(\phi)$ and $\sigma_S(\phi)/\sigma_D(\phi)$, which is the goal of this study. It is clear that $\Delta M = M$ when $\mu_S(\phi) = \mu_D(\phi)$ and that $\Delta M \rightarrow 0$ when the difference between the mean values ($\Delta\mu(\phi) = |\mu_S(\phi) - \mu_D(\phi)|$) increases.

Figure 3 illustrates the contribution of the shape of the distributions $\Delta M(\phi)$ to the Area Metric $M(\phi)$ as a function of the difference between the mean values of the distributions ($|\mu_S(\phi) - \mu_D(\phi)|/\mu_D(\phi)$) and the ratio of the standard deviations of the two distributions $\sigma_S(\phi)/\sigma_D(\phi)$. The four plots present the isolines of $\Delta M(\phi)/M(\phi)$ for four different values of the ratio $\sigma_D(\phi)/\mu_D(\phi)$. The white area of the plots corresponds to $\Delta M(\phi) < 0.01M$.

There is a significant decay of $\Delta M/M$ with the increase of the difference between the mean value of the two distributions. The isolines of $\Delta M/M$ plotted in figure 3 are linear with a slope that depends on $\sigma_D(\phi)/\mu_D(\phi)$. The largest values of $\sigma_D(\phi)/\mu_D(\phi)$ lead to the smallest slopes of the isolines, which means slowest decay of $\Delta M(\phi)/M(\phi)$ with the increase of $\Delta\mu(\phi)$.

The largest value of $\Delta M/M$ is equal to 1 and it is obtained for $\mu_S(\phi) = \mu_D(\phi)$ for any values of $\sigma_S(\phi)/\sigma_D(\phi)$ and $\sigma_D(\phi)/\mu_D(\phi)$. In these conditions ($\mu_S(\phi) = \mu_D(\phi)$), we have $M(\phi) = M_o(\phi)$ with $M_o(\phi)$ defined by equation (4). In order to quantify the filtering of the contribution of the shape of the distributions to $M(\phi)$ for increasing values of $\Delta\mu(\phi)$, figure 4 presents

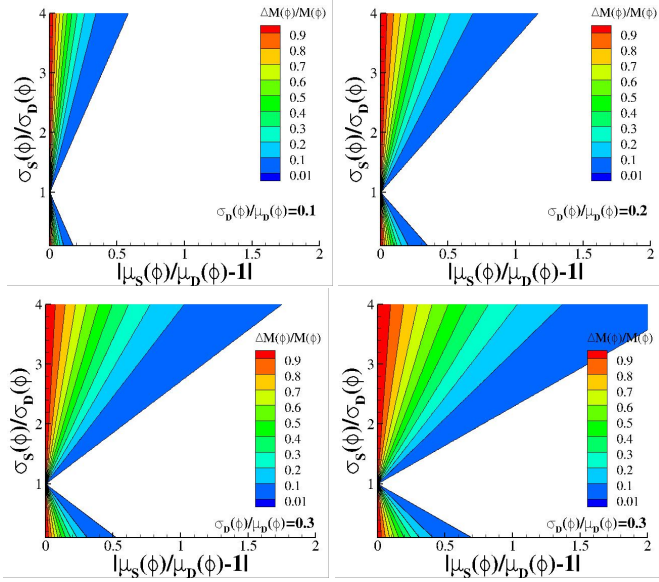


FIGURE 3. Illustration of the contribution of the shape of the distributions $\Delta M(\phi)$ for the value of the Area Metric $M(\phi)$ for normal distributions defining the experimental and simulations results. White area of the plots corresponds to $\Delta M(\phi) < 0.01M$.

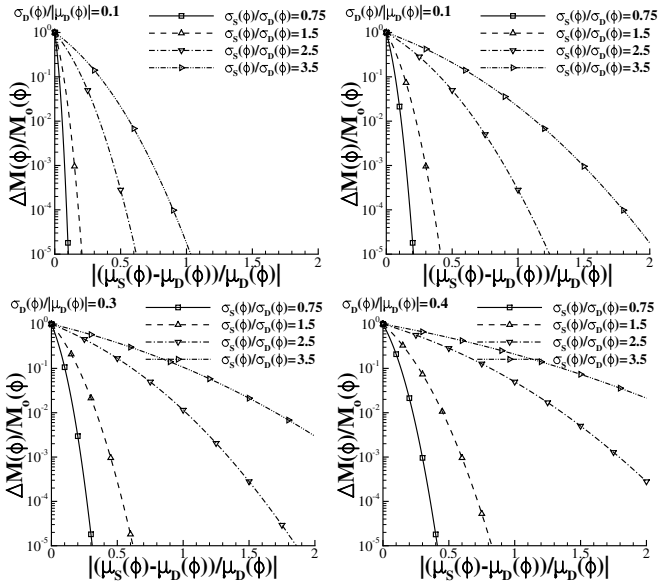


FIGURE 4. Illustration of the decay of the contribution of the shape of the distributions $\Delta M(\phi)$ for the value of the Area Metric $M(\phi)$ for normal distributions defining the experimental and simulations results.

$\Delta M(\phi)/M_o$ as a function of $(|\mu_S(\phi) - \mu_D(\phi)|)/\mu_D(\phi)$ for four values of $\sigma_S(\phi)/\sigma_D(\phi)$ and four values of $\sigma_D(\phi)/\mu_D(\phi)$.

The results show that the contribution of the shape of the distributions can become negligible even for small values $\Delta\mu(\phi)$,

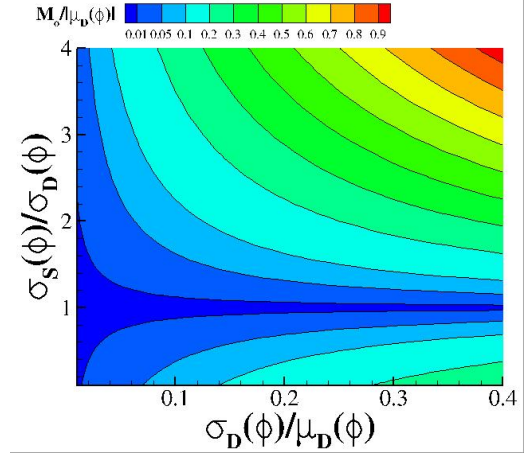


FIGURE 5. Illustration of the contribution of the shape of the distributions $M_o(\phi)$ for the value of the alternative Area Metric $M_a(\phi)$ for normal distributions defining the experimental and simulations results.

which is not a desirable feature for the quantification of modeling errors of stochastic simulations.

3.4 Alternative Area Metric, $M_a(\phi)$

The alternative Area Metric defined by equations (3) to (5) is straightforward to calculate, because $M_o(\phi)$ corresponds to $M_\sigma(\phi)|\mu_D(\phi)|$ when $\phi_I = \mu_D(\phi)$. This leads to

$$\frac{M_o(\phi)}{|\mu_D(\phi)|} = \left| \frac{\sigma_D(\phi)}{\mu_D(\phi)} \sqrt{\frac{2}{\pi}} \left(1 - \frac{\sigma_S(\phi)}{\sigma_D(\phi)} \right) \right|. \quad (14)$$

Figure 5 presents $M_o(\phi)/|\mu_D(\phi)|$ as a function of $\sigma_D(\phi)/|\mu_D(\phi)|$ and $\sigma_S(\phi)/\sigma_D(\phi)$. As desired, the alternative area metric reflects the increase of differences between $\sigma_S(\phi)$ and $\sigma_D(\phi)$ independently of $\Delta\mu(\phi)$.

4 ASME V&V10.1 EXAMPLE

4.1 Problem definition

The validation exercise described in [9] is an elastic, hollow, tapered, cantilever, box beam under a uniform loading applied over half the length of the beam. The quantity of interest is the transverse tip deflection of the beam w , which in the experimental apparatus is measured directly using a displacement transducer. Details of the geometry are given in [9], including the constraints to apply at the “fixed-end” of the beam, where the rotational constraint is assumed to vary linearly with the magnitude of the moment reaction. For the sake of clarity, the problem is illustrated in figure 6.

In the V&V10.1 standard [9], two different approaches are presented: one that uses one single experiment compared to

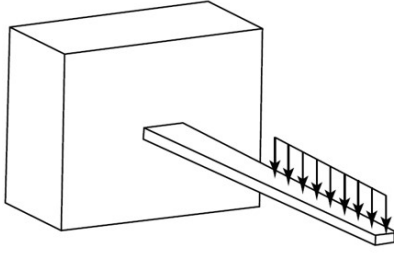


FIGURE 6. Schematic of the Hollow Tapered Cantilever Beam [9].

one simulation with all possible uncertainties involved estimated from subject matter experts, or one that uses a modeling error assessment based on 10 replicate experiments using 10 nominally identical beams and additional sets of experiments to characterize the two random input variables, the modulus of elasticity of the beam material Y and the flexibility of the linear rotational spring restraining the beam at its constrained end f_r . Results for the first approach based only on expert opinion are not addressed in this paper.

4.2 Experimental data

Experimental measurements are assumed to have a negligible experimental uncertainty (random or systematic), but there is variability in the results due to the material properties³ Y and f_r .

The results of the experiments performed for the 10 nominally identical beams are presented in [9] and are not reproduced in this paper. Nonetheless, the discrete PDF and CDF derived from the 10 experimental measurements of the beam-tip deflection are plotted in figure 7. The plot also contains the PDF and CDF of a normal distribution with the same mean value⁴ $w_{\text{mean}}^{\text{exp}} = -15.36(\text{mm})$ and standard deviation $\sigma_{w^{\text{exp}}} = 0.568(\text{mm})$ of the discrete PDF.

The CDF obtained from the normal distribution fitted to the data of the 10 experiments is in reasonable agreement with the discrete CDF taking into account the relatively small number of samples.

4.3 Simulations data

The simulations are based on the numerical solution of the equation of static Bernoulli-Euler beam theory, which requires the experimental values of the modulus of elasticity of the beam material Y and the flexibility of the (conceptual) linear rotational spring restraining the beam at its constrained end f_r . Beam geometry and loading are assumed to have exact values.

³ f_r actually depends on installation variability (as discussed in [9]) as well as on Y , which in [9] is designated by E .

⁴The results are reported in [9] with only 3 significant digits for the mean value and 2 significant digits for the variance.

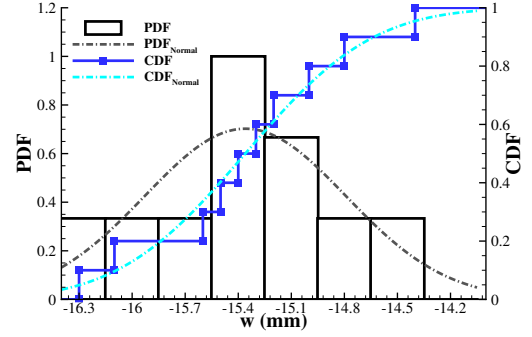


FIGURE 7. Discrete probability density function (PDF) and cumulative distribution function (CDF) derived from the 10 experimental measurements of the beam-tip deflection. $\text{PDF}_{\text{Normal}}$ and $\text{CDF}_{\text{Normal}}$ of a normal distribution with the same mean value and standard deviation of the discrete PDF. Discrete PDF is obtained with $\Delta w = 0.3\text{mm}$.

Grid refinement level⁵ and machine precision are sufficient to guarantee a negligible contribution of the numerical uncertainty.

The modulus of elasticity Y of the material used in the beam and the rotational flexibility, f_r , at the clamped end of the beam are defined by probability density functions that are obtained from independent experiments. Details on the determination of the PDF's that characterize Y and f_r are presented in [9]. For the present exercise, the only important information is that any errors in the determination of these normal distributions (small number of samples, selected distribution, measurement errors,...) are assumed (following [9]) to be negligible and so they do not influence the estimation of the modeling error of the quantity of interest.

The Monte Carlo method used “a large number of samples” [9] to propagate the Y and f_r distributions through the mathematical/computational model. The implied statistical convergence is also sufficient to ensure a negligible level of uncertainty in the simulation results. This means that variability in the simulation results is dominated by the variability in Y and f_r , which matches the conditions of the experimental data.

Figure 8 compares the CDF presented⁶ in [9] with the CDF defined by a normal distribution obtained from the reported mean value $w_{\text{mean}}^{\text{sim}} = -14.1(\text{mm})$ and standard deviation of $\sigma_{w^{\text{sim}}} = 0.65(\text{mm})$. For illustration purposes, the normal PDF is also plotted in figure 8. The normal distribution is close to the CDF presented in [9] obtained from the Monte Carlo simulations.

⁵Possibly iterative convergence as well, but it is not clear in [9] if the computational model uses any iterative solution technique.

⁶The line plotted is obtained from the plot presented in [9]. The present authors have no knowledge about the exact shape of this CDF.

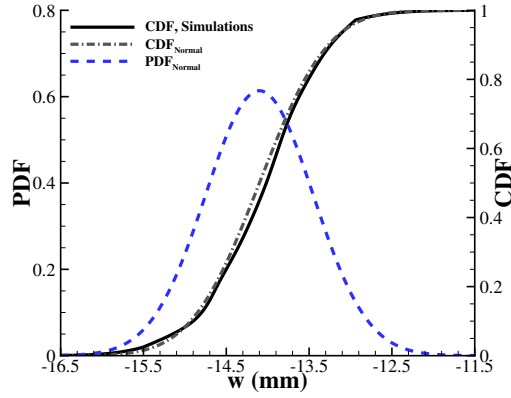


FIGURE 8. Cumulative distribution function CDF presented in V&V10.1 [9] for the computed of the beam-tip deflection w^{sim} . PDF_{Normal} and CDF_{Normal} of a normal distribution with the same mean value and standard deviation of the simulations.

4.4 Area Metric results

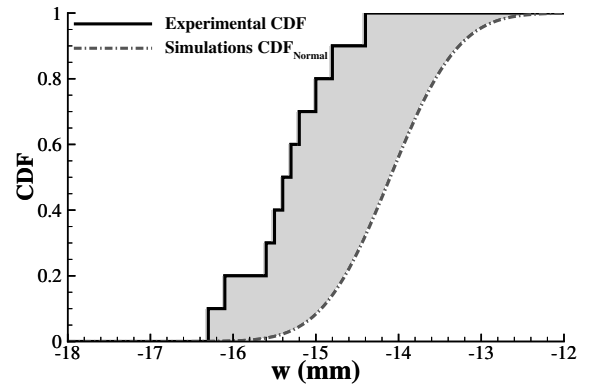
Using the discrete CDF of the experiments and simulations CDF, the result reported in [9] is $M(w) = 1.3(\text{mm})$, which is exactly equal to the difference between the mean values of the two distributions. Therefore, it has a negligible contribution of the different shapes of the experimental and simulations CDF's.

In order to confirm the insensitivity of $M(w)$ to the shape of the distributions, we have performed some extra determinations of $M(w)$ using the normal distribution fitted to the simulations CDF_{Normal} and the discrete and normal CDF's that characterize the experimental data. Figure 9 illustrates the three CDF's used to make the two additional estimates of the Area Metric.

For the bottom plot of figure 9, experimental CDF_{Normal} and simulations CDF_{Normal} , the intersection of the CDF's occurs $w_I = -24.1(\text{mm})$ where the two CDF's are almost identical and so the outcome of the Area Metric for the two normal distributions is $M(w) = 1.265(\text{mm})$. The result obtained from the discrete experimental CDF and the simulations CDF_{Normal} , top plot of figure 9, is $M(w) = 1.260(\text{mm})$, which means that there is a difference of $0.005(\text{mm})$ between the two evaluations of $M(w)$, which corresponds to 0.03% of the mean experimental value of w . Therefore, in these conditions, the Area Metric is nearly insensitive to which CDF is used for the experimental data.

The insensitivity of $M(w)$ in this example was further explored by using for the simulations a CDF defined by a Heaviside function with the step at $\mu_S(w)$ ($CDF_{Heaviside}$). This CDF is obtained from a single simulation using the mean values of Y and f_r that we will assume to lead to approximately the mean value of the stochastic simulations. These evaluations of $M(w)$ are illustrated in figure 10 and the results obtained are $M(w) = 1.260(\text{mm})$ for the discrete experimental CDF and $M(w) = 1.304(\text{mm})$ for the normal distribution fitted to the experimental data. These results are equal to those obtained with

Discrete Experimental CDF and Simulations CDF_{Normal}



Experimental CDF_{Normal} and Simulations CDF_{Normal}

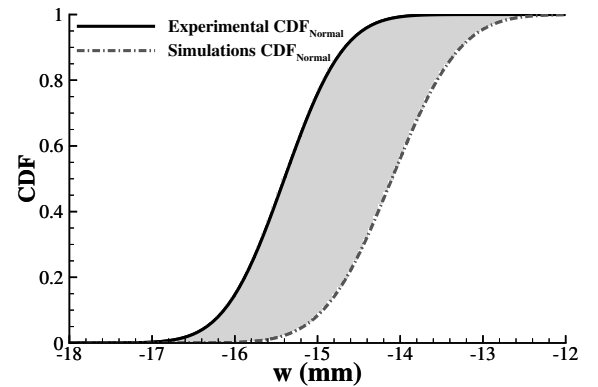


FIGURE 9. Cumulative density functions (CDF) of the simulations and experiments for additional estimations of $M(w)$ using discrete and normal distributions for the experimental CDF and a normal distribution for the simulations CDF in the example of [9].

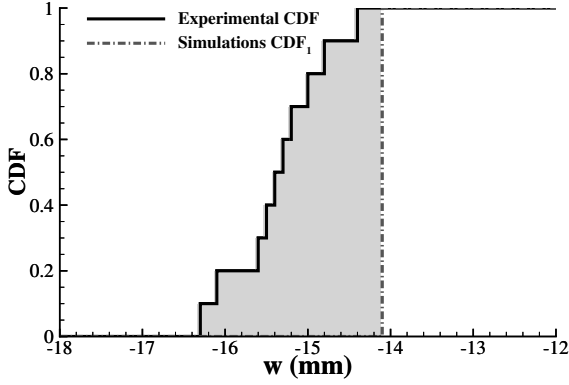
TABLE 1. Area Metric evaluations for the quantity of interest of the example of V&V10.1 using different approximations of the experimental and simulations CDF's.

Experimental CDF	Simulations CDF	$M(w)$ (mm)
Discrete	[9]	1.3
Discrete	Normal	1.260
Discrete	Heaviside	1.260
Normal	Normal	1.265
Normal	Heaviside	1.265

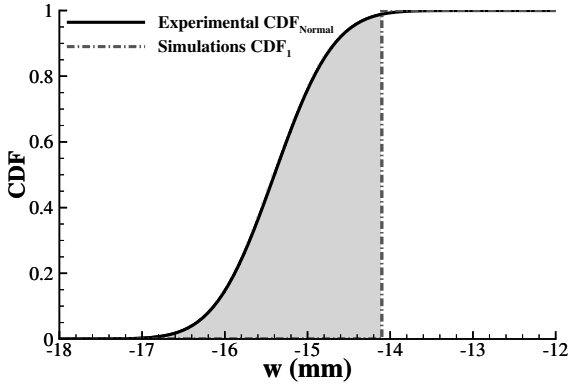
the normal distribution fitted to the results of the stochastic simulations.

Table 1 summarizes all the evaluations of $M(w)$ illustrated

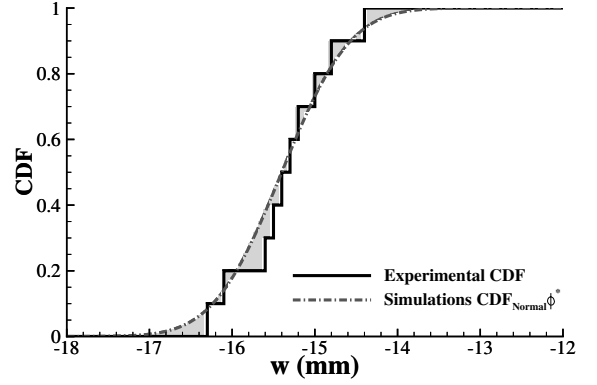
Discrete Experimental CDF and Simulations CDF_{Heaviside}



Experimental CDF_{Normal} and Simulations CDF_{Heaviside}



Discrete Experimental CDF and Simulations CDF_{Normal}



Experimental CDF_{Normal} and Simulations CDF_{Normal}

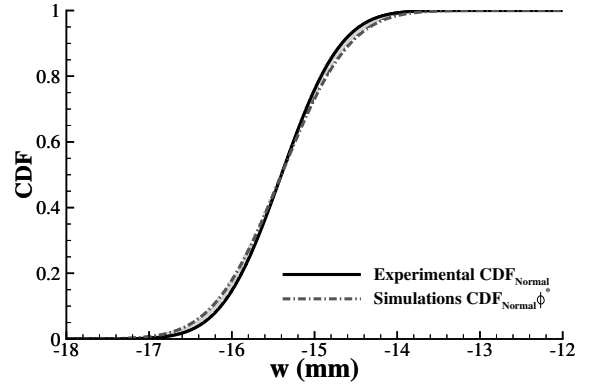


FIGURE 10. Cumulative density functions (CDF) of the simulations and experiments for additional estimations of $M(w)$ using discrete and normal distributions for the experimental CDF and an Heaviside distribution for the simulations CDF in the example of [9].

FIGURE 11. Cumulative density functions (CDF) of the simulations and experiments for the estimations of the alternative Area Metric $M_a(w)$ using discrete and normal distributions for the experimental CDF and a normal distribution with the experimental mean value for the simulations CDF in the example of [9].

in figures 9 and 10. Although significantly different CDF's were tested, including a CDF obtained from a single simulation, the values are all almost equal to the difference between the mean values of the experiments and simulations. Therefore, in the V&V10.1 example, the Area Metric is insensitive to the shape of the experimental and simulations distributions and so it cannot be an appropriate metric for Validation exercises of stochastic simulations.

4.5 Alternative Area Metric results

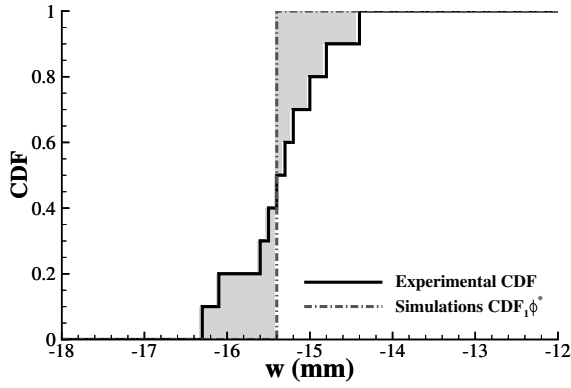
The alternative Area Metric is tested using the discrete and normal CDF's of the experiments and the normal and Heaviside CDF's of the simulations, as illustrated in figures 11 and 12. The values obtained for $M_a(w)$ are presented in table 2. We recall that the gray area of the plots of figures 11 and 12 corresponds to the contribution of the different shapes of the distributions $M_o(w)$ to the value of $M_a(w)$.

TABLE 2. Alternative Area Metric evaluations for the quantity of interest of the example of V&V10.1 using different approximations of the experimental and simulations CDF's.

Experimental CDF	Simulations CDF	$\mu_S(w) - \mu_D(w)$ (mm)	$M_o(w)$ (mm)	$M_a(w)$ (mm)
Discrete	Normal	1.26	0.068	1.328
Discrete	Heaviside	1.26	0.370	1.630
Normal	Normal	1.26	0.066	1.326
Normal	Heaviside	1.26	0.453	1.713

With the simulations represented by a normal distribution CDF_{Normal}, the alternative Area Metric is 5.40% larger than the

Discrete Experimental CDF and Simulations CDF_{Heaviside}



Experimental CDF_{Normal} and Simulations CDF_{Heaviside}

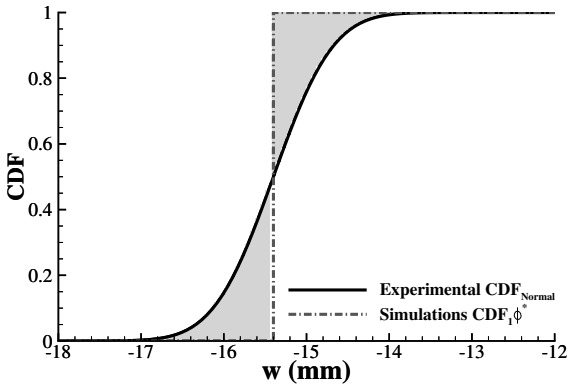


FIGURE 12. Cumulative density functions (CDF) of the simulations and experiments for the estimations of the alternative Area Metric $M_a(w)$ using discrete and normal distributions for the experimental CDF and a Heaviside distribution with the experimental mean value for the simulations CDF in the example of [9].

original $M(w)$ for the discrete experimental CDF and 4.82% larger than the original $M(w)$ for the experimental CDF_{Normal}. The use of a single simulation leads to a significant increase of $M_a(w)$, as illustrated in figure 12. For the discrete experimental CDF, $M_a(w)$ is 29.4% larger than $M(w)$ and for the experimental CDF_{Normal} $M_a(w)$ is 35.4% larger than $M(w)$. Thus the alternative Area Metric reflects the different shapes used for the experimental and simulations CDF's. Furthermore, as expected, it shows a significant increase for the single simulation CDF_{Heaviside}.

The alternative Area Metric provides more than a single number $M_a(w)$. As illustrated in table 2, it gives a difference between the mean values of the two distributions (that does not have to be the absolute value) and an evaluation of the difference between the shapes of the two distributions $M_o(w)$. Naturally, the same approach can be applied to the original Area Metric using equation (13) to determine $\Delta M(w)$. However, as demonstrated in the previous section, the value of ΔM tends

very rapidly to zero with the increase of $\Delta\mu$. The three ratios that control the value of $M(w)$ for normal distributions are $|\mu_S(w) - \mu_D(w)|/|\mu_D(w)| = 0.082$, $\sigma_D(w)/|\mu_D(w)| = 0.037$ and $\sigma_S(w)/\sigma_D(w) = 1.14$. For these settings, the plots of figures 3 and 4 explain the insensitivity of $M(w)$ to the shape of the distributions obtained for the example of [9].

5 CONCLUSIONS

This paper discusses the use of the Area Metric for Validation exercises of stochastic simulations. The examples used in this work assume (following [9]) the ideal conditions for the application of this metric: uncertainty in the experimental and simulations results for the quantity of interest depend only on the variability of material properties. This means that experimental measurement uncertainty, numerical uncertainty, statistical uncertainty and any uncertainties in the definition of the input parameters probabilistic distributions are negligible. In this idealized setting, the Area Metric is supposed to quantify the modeling error of a quantity of interest determined by a stochastic simulation.

The simple examples included in this study lead to the following conclusions:

- The original Area Metric becomes insensitive to the shape of the experimental and simulations probabilistic distributions even for small differences between the mean values of the two distributions. Naturally, the filtering of the distributions shape influence depends on the ratio between the standard deviation and mean value of the experiments and on the differences between the shapes of the experimental and simulations distributions.
- For the conditions of the example presented in V&V10.1, the original Area Metric is nearly insensitive to the shape of the experimental and simulations distributions. It leads to an evaluation of the modeling error equal to the simple difference between the mean values of experiments and simulations, which is an unacceptable result even for validation exercises of deterministic simulations.
- An alternative formulation of the original Area Metric is proposed in this paper. The contribution to the estimate of the modeling error of the difference between the shapes of the experimental and simulations distributions is independent of the difference between the mean values of both distributions.

Last but not the least, it must be mentioned that the estimation of modeling errors in practical engineering problems where most of the assumptions used in the examples of this paper are not valid (following [9]) is an huge challenge for any Validation metric.

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