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Validation and verification of nonlinear mechanical models for nuclear buildings and equipment: an application

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ABSTRACT

Due to the increasing complexity of numerical models in mechanics, it is more and more difficult to ensure the validity of simulation results and therefore the reliability of the consecutive decision making. Several definitions, guides and norms have been published during the last decades regarding the good practices in the field of "Validation & Verification" (V&V). However, none of them really propose a clear and straightforward applicable method to perform validation and verification of a nonlinear numerical mechanical model. IRSN[1] and EDF[2] decided to work within a joint framework aiming at defining more precisely the V&V concepts and related declinations. The choice is made here to focus on examples of practical applications of V&V guidelines. The authors believe that such examples will bring more clarity than general concepts, even if the latter remain essential as references. First, the main concepts are defined and are placed in connection with the works carried out by various institutions and research teams to define a general V&V framework. Second, the aforementioned concepts are applied to the pragmatic practical case of two pounding structures. Finally, the perspectives of the V&V IRSN-EDF joint work are presented.

INTRODUCTION

Facing to the increasing safety requirements of nuclear structures and equipment, it is crucial to have tools or procedures to justify the use of newly developed nonlinear model, *i.e.*, to verify the numerical implementation of the mathematical model, the software quality assurance, with auditable calibration and documentation (**Verification**), and to assess the needed sufficient accuracy in representing the actual physical responses within the expected application range for the safety demonstration (**Validation**). This is of primary importance since it allows improving the confidence level of safety margin assessment.

In this context, IRSN and EDF decided to work together within a joint framework aiming at interpretating the validation & verification (V&V) in the context of civil engineering and nuclear safety. As shown by Figure 1, several definitions, guides and norms have been published during the last decades such as the ones by the American Institute of Aeronautics and Astronautics (AIAA) and the French Nuclear Safety Authority (ASN). However, these guidelines are rather compendiums of good practices and overall objectives, but none of them really propose a clear and straightforward applicable method to perform validation and verification of a nonlinear numerical mechanical model. Schwer (2007) notably recognized

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that a step-by-step *standard* is many years in the future. V&V topics have been studied in various scientific fields notably by American research teams such as Sandia laboratory.

Figure 1. Publication years of the main guides in the field of V&V

Thus, the main goal of this work is to take a survey of current practices, both from a regulatory and research point of view and to propose several comprehensive, practical and pragmatic industrial applications of state-of-the-art V&V methods. The authors believe that such examples will bring more clarity than general concepts, even if the latter remain essential as references. EDF and IRSN first designed consensually a procedure (composed of two verification and validation sections) inspired from the literature for engineering purposes. The choice has been made to create a rather general approach because accounting for the high diversity of scientific domains and modelling strategy would results in an unusable and over-

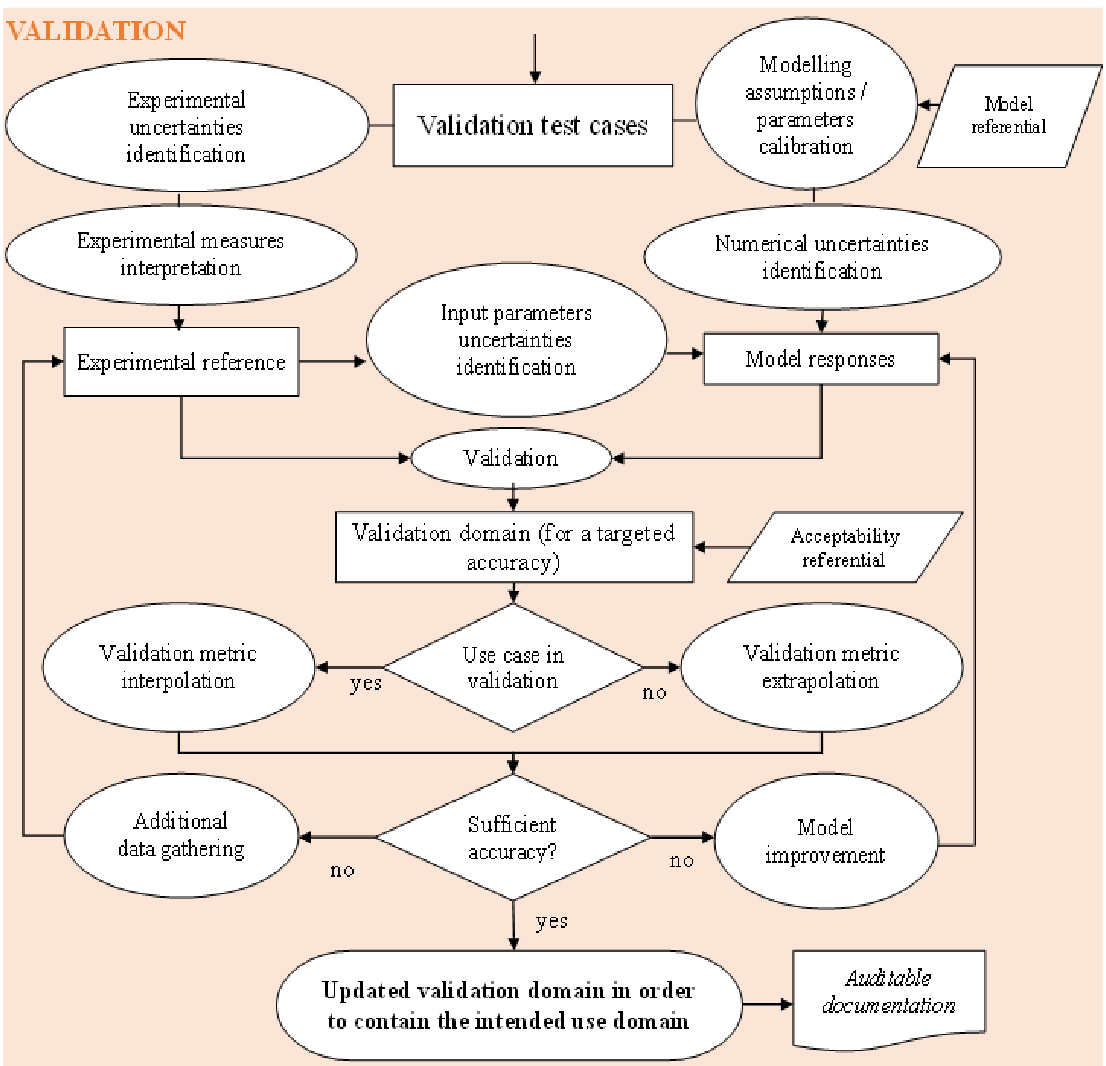

Figure 2: Validation diagram

complexed diagram. Figure 2 presents the resulting product for validation, inspired by Trucano et al. (2001), Thacker et al. (2004), Oberkampf and Barone (2006), Kats and Els (2012).

The verification process may be associated with adapted computer development and quality insurance practices. For the sake of simplicity, a focus is made in this paper on the validation process only which intervene after the verification one. The works by Roy and Oberkampf (2011) highlighted the importance of uncertainties in the validation process, which was accounted for during the diagram design. The validation process can be applied in an experimental versus numerical comparison, or in a numerical simplified model versus numerical reference model. In the first case, this allows to directly confront the numerical output to the experimental data. If such measures are not available, the procedure can be applied with a refined reference model considered as a numerical experiment. Uncertainties are introduced in this model to reproduce experimental variability and obtain *pseudo-experimental* results. Then, a simplified (less refined for instance) model is calibrated accordingly. This allows for a comprehensive monitoring of input and measure uncertainties or operating conditions that could blur the reasons of the mismatch between the model and the reference.

In the following, the Validation diagram is applied to the numerical versus experimental case of two structures subjected to earthquake-induced structural pounding. Finally, the perspectives of the V&V IRSN-EDF joint work are presented.

VALIDATION TEST CASES

This section presents the experimental set-up, properties, input, and output at our disposal. Only the essential information are detailed here, for two reasons: (1) simplicity; (2) the validation process itself does not require much details and the model may be regarded as a “black box”. The PhD thesis by Crozet (2019) enabled the study of two adjacent 2.4m high single-storey structures (named 1 and 2) embedded on a shaking table (displayed by Figure 3). The slabs are made of reinforced concrete and the columns are steel made, the objective being to keep them in their elastic state. The separation distance, *i.e.* the gap equals 2 cm, and the ratio of their periods equals averagely 0.55, to ensure pounding occurrences. They were subjected to 23 ground motions of various intensities (Table 1), and multiple sensors allowed to register the displacements and accelerations. The Structural Response Quantity (SRQ) of interest is the interstorey-drift δ of Structure 1 and 2, respectively δ_1 and δ_2. It is a common response parameter for engineers to study during design stages of buildings. It is calculated here by dividing the maximum floor displacement by the interstorey-height. Other SRQs such as the floor response spectra could have been investigated.

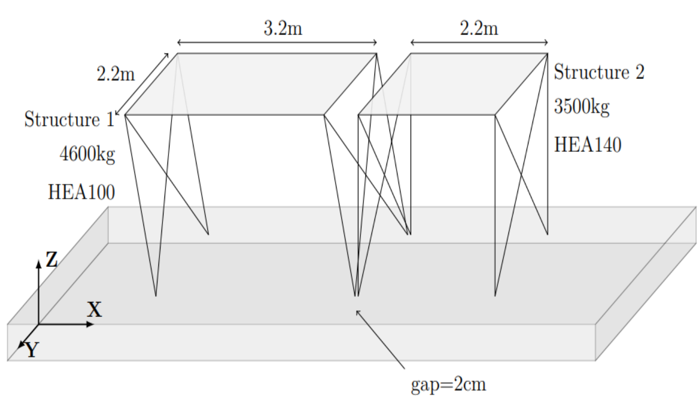

Figure 3: Scheme of the single-storey structures

Table 1: List of ground motions

Ground Motions involving impact (Number of tests)	**Peak Ground Acceleration during the tests (PGA) (g)**
Cadarache (2)	≈ [0,28 0,30]
El Centro (4)	≈ [0,35 0,40]
Northridge (10)	≈ [0,32 0,42]
Kobe (7)	≈ [0.37 0,43]

EXPERIMENTAL MEASUREMENTS AND UNCERTAINTIES

This section presents the various steps in assessing which are the experimental uncertainties and to interpret the measures. This section comes naturally before the numerical computation of the model which will account for these uncertainties. An important aspect of this section is that the consultation of experts resulting in a consensual decision to move a step forward seems preponderant. A diagram alone cannot estimate, from one application study to another, which uncertainty should be investigated.

Interpretation of experimental measures

Earthquake-induced building pounding is a phenomenon involving multiple parameters. Indeed, not only one but at least two structures are considered, increasing consequently the number of variables and potential discrepancies. In the campaign by Crozet (2019), it was shown that it is difficult to keep the structures motions only in the longitudinal direction as desired, as torsion motion was triggered on several occasions. Tests are also not easily repeatable, as subjecting the structures two times to the same ground motion input can result in significantly different occurrences of collisions, and consequently changing the structural response. These discrepancies can come from uncertainties in the seismic input through the shaking table, a different separation distance between each test, or a misalignment of the slabs. SRQs can consequently vary significatively from one test to another, even for identical input signals and experimental setups.

Identification of experimental uncertainties – Consequences on model input parameters

The goal here is to assess which variable are the most uncertain and have the most influence on the results. Experts' judgements and sensitivity analyzes are here paramount to make the better choices. As in Roy and Oberkampf (2011), uncertainties can be either *epistemic* (due to a lack of knowledge, characterized by an interval) or *aleatory* (due to an inherent variability of the observed quantity, characterized by a distribution function).

First, the gap separation between the structures is considered as an epistemic uncertainty as there are no insurance that it is perfectly 2cm for each test. A uniform distribution is consequently set for this variable, and a Latin hypercube of five samplings between 1.9cm and 2.1cm will be applied.

Secondly, the aleatory uncertainty was debated either between either the two damping coefficients ξ_1 and ξ_2 (greater than 0%) respectively for Structure 1 and Structure 2, or the collision treatment dealt numerically by the coefficient of restitution e (contained between 0 and 1) of the Non-Smooth Contact Dynamics Method (NSCD) developed by Acary (2008), and used in Langlade (2021a, 2021b). For simplicity and computation time costs reasons, only one variable was retained as an aleatory uncertainty. To decide which one to use as uncertainty, a sensitivity analysis and/or expert judgement is necessary to investigate how much the SRQs are influenced by these parameters, and how well they can be assessed. Thus, the consideration of the nature and level of design of the numerical model is already important and to be considered in this stage of identification and quantification of the uncertainties.

NUMERICAL MODELLING AND UNCERTAINTIES

Model referential

The model referential refers to the software, experience, and numerical tools at disposal. In the present case, to achieve structural dynamic analyzes involving collision, the choice was to use the NSCD method implemented in the **ATL4S** platform built by Grange (2021). Since this article is a first introduction to the V&V process, the choice was made to use a planar model, with Euler-Bernoulli beam elements.

Now, this numerical model needs to be sufficiently refined to ensure an accurate assessment of ξ_1, ξ_2, and *e* by using the experimental output, as well by yielding such results with a reasonable computation time.

Numerical uncertainties - Choice of the numerical model

Herein, six planar frame models with 3, 6, 12, 24, 48, and finally 96 elements are considered. They are subjected to the 23 ground motions and the SRQs δ_1 and δ_2 are studied. Following the work by Langlade (2021), the coefficients ξ_1, ξ_2, and *e* were temporarily set to 0.6%, 0.5% and 0.6. It appeared that despite some cliff effects inherent to pounding phenomenon, refinement has no systematic influence beyond the 6-element model. Thus, numerical uncertainties are neglected. Because the computations runtimes are short considering the behaviour is elastic, the 12 elements-frame model was selected to assess of ξ_1, ξ_2, and *e*.

VALIDATION METRICS AND PARAMETERS CALIBRATION

This section presents how the distribution of ξ_1, ξ_2, and *e* coefficients are evaluated, and which one will be eventually considered as aleatory. Again, the experts' role is necessary to evaluate the means and time necessary to calibrate the parameters considering the knowledge already gathered on them. Langlade (2021) assessed that ξ_1, ξ_2, and *e* were respectively equal to 0.6%, 0.5%, and 0.6 but it was a qualitative assessment, with a different numerical model, and using only six pullback tests[3] out of the 16 from Crozet (2019) experiments. Thus, to have a more complete study and quantitative assessment of ξ_1, ξ_2, and *e*, it is possible to use a metrics such as the Russel or the Sprague & Geers metrics as in Kats and Els (2012). Also, not only the six but the whole set of 16 pullback tests data can be used for the numerical parameter calibration.

Russel metrics R_u

Russel and Sprague&Geers metrics, respectively named R_u and SG, are adapted to measure differences between two time-history series because unsensitive to divisions by zero. They are greater than or equal to zero, have no units. The numerical output vector is evaluated against a reference/experimental vector in terms of magnitude M_R and phase P_R. Both vectors should have the same dimension. Equations (1), (2), (3), and (4) display successively how R_u is computed. SG metric differs from R_u only *via* the phase term.

$$rme = \frac{\Sigma_{i=1}^{N} p_i^2 - \Sigma_{i=1}^{N} m_i^2}{\sqrt{\Sigma_{i=1}^{N} p_i^2 * \Sigma_{i=1}^{N} m_i^2}} \tag{1}$$

$$M_R = \operatorname{sign}(rme) * \log(1 + |rme|) \tag{2}$$

$$P_R = \frac{1}{\pi}\cos^{-1}\left(\frac{\Sigma_{i=1}^{N} p_i m_i}{\sqrt{\Sigma_{i=1}^{N} p_i^2 * \Sigma_{i=1}^{N} m_i^2}}\right) \tag{3}$$

$$R_u = \sqrt{\frac{\pi}{4}(M_R^2 + P_R^2)} \tag{4}$$

Where m_i and p_i are respectively the measured and computed points.

Metrics allow a relative comparison between various candidate vectors and the reference, but it is of interest to have a more absolute approach, *i.e.*, for a given value of R_u, the comparison is considered either satisfying or insufficient. Thus, a two-second sinus vector (unitary amplitude and period) is plotted in thick black line in Figure 4 and considered as the experimental /reference data. Three other series are considered, one with an amplitude 20% greater than the reference's (green curve), one with an out-of-phase motion of $-\pi/8$ (blue curve), and the last one combining the two latter discrepancies (red curve). These

[3] Structure 1 is pulled backwards, released, and goes pounding against Structure 2 in a free motion state.

values were chosen purely arbitrarily by the authors because considered as "limit cases" where civil engineers judge a comparison satisfying enough or not. As expected, R_u metrics applied to the reference vector itself yields a zero value. The highest value R_u=0.173 falls on the red curve as expected as being the combination of the two other errors and can potentially serve as an absolute criterion. One must point out that R_u and $S\&G$ metrics are independent from time discretization and length of the signal.

Area validation metric d (L_1 norm - Minkowski norm))

The area validation metric, also named L_1 or Minkowski norm, is particularly fitted when comparing a numerical Cumulative Density Function (CDF) with a reference CDF. Their dimensions can be different. Equation (5) displays d formulation and Figure 5 its graphic interpretation.

$$d(F, S_n) = \int_{-\infty}^{+\infty} |F(x) - S_n(x)| \cdot dx \quad (5)$$

Where F and S_n are respectively the numerical and experimental CDFs. d is greater than or equal to zero and has the peculiarity to have the same unit than the data studied.

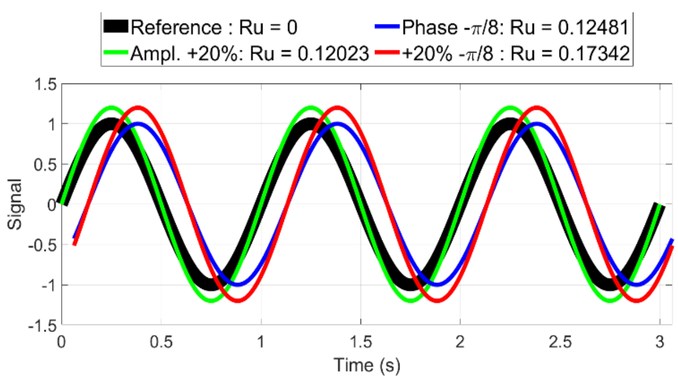

Figure 4: Russel metrics example

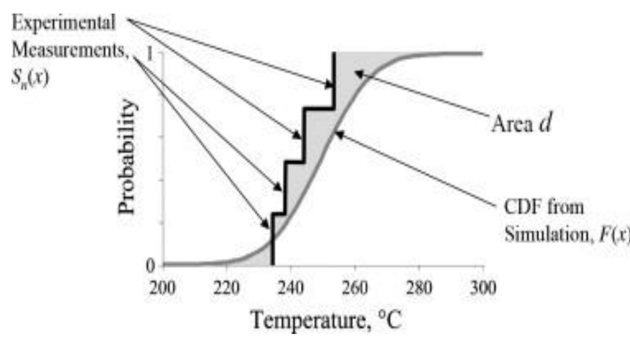

Figure 5: Area metric d illustration from Roy and Oberkampf (2011)

Assessment of ξ_1, ξ_2, and e

To assess ξ_1, ξ_2, and *e*, the displacements and floor response spectra of the 16 pullback tests available for different values for each of the coefficients. ξ_1 and ξ_2 range is [0 2]% and *e* range is [0 1]. Then, the Russel metrics is computed for each run. The best mean values of ξ_1 and ξ_2 were found to equal 0.4 % and 0,5 %, while *e* = 0.7 yielded the smallest Russel values as shown by Figure 6. A sensitivity analysis, such as in Crozet (2017), should be applied to evaluate how much the SRQs vary relatively to the different parameters of the NSCD method. Conversely, the authors decided to set deterministically the values of the ξ_1 and ξ_2, and to choose the coefficient of restitution *e* as the aleatory variable with a normal distribution of mean 0.7 and standard deviation 0.1. This enables shorter computations as only one variable is considered, instead of two or three. A Monte-Carlo of 50 samplings is computed for each of the five gap separation values.

INPUT AND MODEL UNCERTAINTIES IN THE VALIDATION DOMAIN

Experimental reference

The experimental reference sets the experimental frameworks, hypothesis, conditions, and output of the study. For instance, in the present case, despite knowing that transversal motion occurred repeatedly over various tests, the authors stipulate that the system remains globally plane, and that the structures can be modelled perfectly aligned. This allows to model a 2D system instead of a 3D. The frequencies (3.55 Hz and 6.55 Hz) and masses (4.6 tons and 3.5 tons) are taken as given by Crozet (2019). As detailed above, the damping coefficients ξ_1 and ξ_2 are set equal to 0.4% and 0.5%.

Validation domain

The validation domain of the above computations corresponds to a PGA contained between 0.28g and 0.43g. Obviously, any other relevant intensity measure than PGA could have been used for the purpose of the V&V process presentation, such as the pseudo-acceleration Sa calculated at the fundamental period T_f of a particular structure, $S_a(T_f)$. For instance, if the period of Structure 2 were to be chosen, the validation domain would then be [0.56 0.92]g.

Input uncertainties propagation

As in Roy and Oberkampf (2011), for each ground motion, five epistemic values are considered, yielding five CDFs with 50 samplings of *e* drawn for each CDF. From these curves, the widest outline is kept, and called a p-box. Figure 7 illustrates this stage of the process. The five colored dashed lines are the five CDFs generated by their respective 50 Monte-Carlo samplings, for <u>one</u> seismic test of PGA 0.36g. The thick black line draws the respective p-box. Finally, the vertical red line is the measurement δ_1 of the respective seismic test during the experimental campaign.

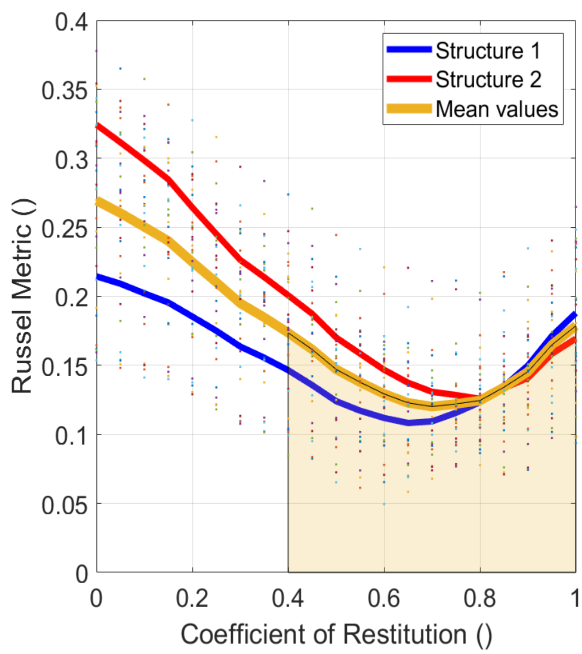

Figure 6: Means of Russel metrics against *e* values calculated for 16 Pullback tests

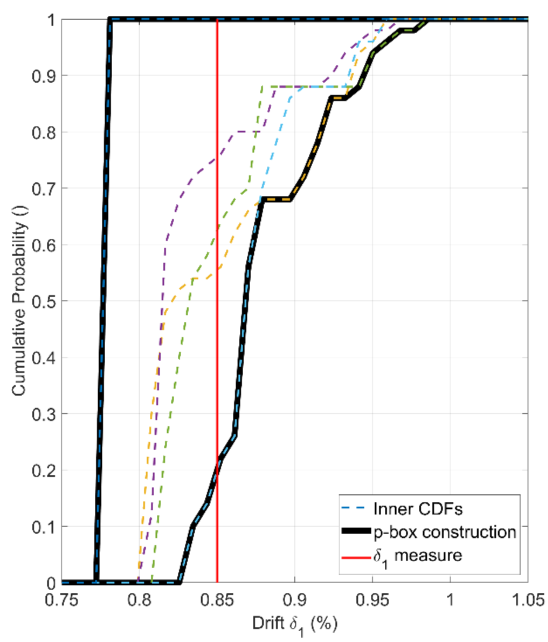

Figure 7 : p-box construction at PGA=0.36g.

At this stage, it is already possible to read the probabilities that δ_1 is over or below a critical threshold, and to give a probability of such occurrence, for a seismic ground motion whose PGA is 0.36g. For instance, for the numerical model used and by combining the epistemic and aleatory uncertainties, there is 95% probability that δ_1 is greater than 0.77% and smaller than 0.95%. It is also possible to analyze qualitatively and comprehensively the variables effects on the SRQ of interest. First, the left p-box border is vertical, showing that e has not influence here unlike the other CDFs. This shows that there is probably no collision occurrence for this gap separation value, corresponding to 2.1cm here. For smaller separation distances, δ_1 increases, showing that pounding is detrimental to structural capacity for this study case.

Model form uncertainty

If the p-box shown in Figure 7 contained completely the measurement (red line), then the model would not need significant further improvement, and there would be no uncertainty due to the model form. Conversely here, there is still room for model improvement as this p-box only envelops partially the measurement. Model modification could be performed until the 23 measurements are captured altogether but this might result cumbersome, especially considering the cliff effects inherent to building pounding phenomenon.

Rather than modifying the numerical model, Roy and Oberkampf (2011) estimated the model form uncertainty by computing the area validation metrics d (see Figure 5) for each of the 23 tests and interpolate or extrapolate d inside or outside the validation domain (here, between [0.28 0.43] g). This metrics serves then as model form uncertainty as it has the same units than the SRQ of interest. In the example above, d is computed, equals 0.02%, and can be accounted for with the input uncertainties. A visual example of combination of both input and model uncertainties for a given PGA will be given in the following section.

Figure 8 displays the d metrics of the 23 seismic tests respectively for Structures 1 (blue dots) and 2 (red dots). To estimate the model form uncertainty over the domain, these authors computed a linear regression (thick dashed lines) as well as a confidence 95% prediction interval (thin lines) with a Student distribution. It is then possible, for a given PGA, to assess both the model and the input uncertainties. Depending on the number of experimental measures, their trend, the phenomenon represented, and on the expert recommendations, any other type of regression and prediction interval could be used.

EXTRAPOLATION TO AN INTENSITY MEASURE OUTSIDE THE VALIDATION DOMAIN

Model input uncertainty outside the validation domain

If a SRQ is sought at a given intensity measure outside the validation domain where no experimental data is available, *e.g.*, PGA=0.6g, the input uncertainties should again be calculated. Because the structural response to two different ground motions with a same PGA can be significatively different, the authors decided to account for such variability. A set of 1000 different ground motions has been selected and scaled at a PGA of 0.6g, under the assumption that the resulting seismic input remains realistic. As before, the p-box at 0.6g is computed with five epistemic separation distance values, and for each with a Monte-Carlo technique of 200 samples this time, each sample corresponding to an individual ground motion and coefficient of restitution e. Figure 9 presents the resulting p-box drawn as the blue area.

Model form uncertainty outside the validation domain

The Student distribution method abovementioned allows to calculate the model form uncertainty also outside the validation domain. It is then possible to account for the induced additional uncertainty of the extrapolation to 0.6g. The prediction yields then the values 0.30% and 0.46% respectively for δ_1 and δ_2, which is considerably high due to the important data scatter. Again, the recommendations of experts are important here to decide which prediction/conservatism interval to apply. For instance, one could have assumed that taking the maximal model form uncertainties calculated in the validation domain (respectively 0.19% and 0.25%) would be conservative enough. In Figure 9, the green area represents the additional model form uncertainty of 0.30% for δ_1 yielded by the prediction displayed in Figure 8.

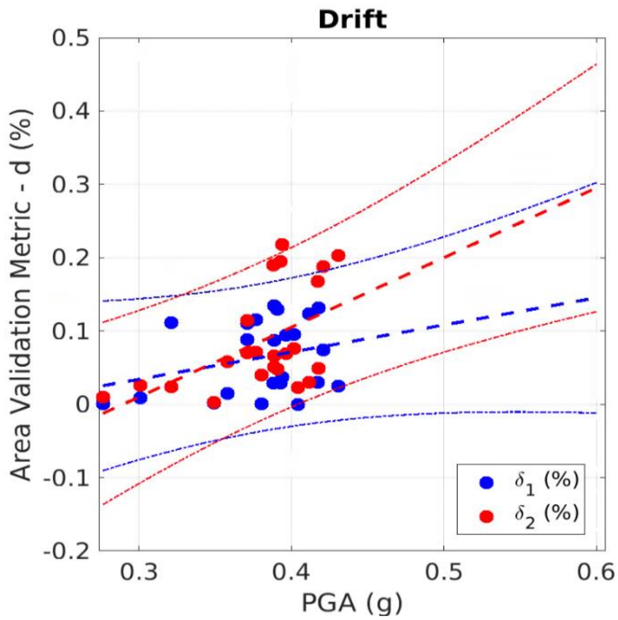

Figure 8: 95% prediction interval over the validation domain and spread to the conditions of interest

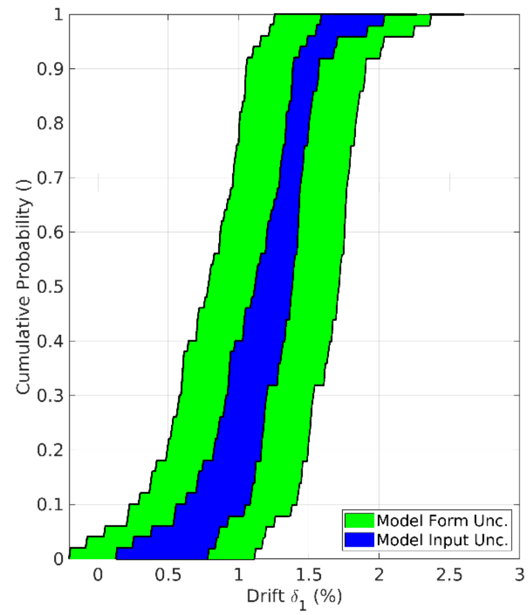

Figure 9: PGA=0.6g. Input form: blue range. Model form: green

Combination of the uncertainties

The combination of the uncertainties is plotted in Figure 9. Here, because building pounding is a phenomenon whose consequences are difficult to estimate due to important cliff effects, the resulting uncertainty box is significantly wide, especially regarding the model form uncertainty extrapolated at 0.6g. For instance, there is a 90% chance that δ_1 is contained between 0.25% and 1.9%. As a reminder, the numerical ones are neglected, otherwise an extra area would appear and widen again the p-box.

CONCLUSION

The V&V process designed by EDF and IRSN aims at a better liability in the implementation of numerical simulations for the safety demonstration, in particular in the range of nonlinear finite elements analyses. A particular topic consists of identifying and quantifying the uncertainties of a system and numerical model to give a probabilistic estimation of the output of interest. It has been tested in the building pounding framework for example purposes but is meant to be addressed to other engineering applications. Overall, and as discussed from the beginning, a process alone cannot drive any study, and the step-by-step experts' recommendations are mandatory, as studies diverge quickly in terms of system, measures, model strategy, objectives. Indeed, other strategies and techniques could have been used during this work (3D modelling, considering other uncertainties, other intensity measures such as S_a, other techniques of regression, etc.). The key limitations to Monte-Carlo simulations originates from the computation times, especially when considering nonlinearities. Then, the abilities to perform fast sensitivity analyzes and extrapolation techniques are necessary to better understand the system, reduce its size, and predict its response. Justified conservatism strategies can also reduce the runtimes by limiting/cancelling Monte-Carlo simulations.

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