Framework for Assessment of Technology Maturation Using Uncertainty Quantification

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The results in this paper come from a project to develop an Uncertainty Quantification (UQ) framework to assist researchers in technology development and maturation. This framework aims to re-frame technology maturation as a process of reducing quantifiable uncertainty instead of completing requirements on a Technology Readiness Level (TRL) scale. The framework provided in this paper uses Bayesian statistics to redefine the technology maturation task as a process of reducing uncertainty in system inputs and outputs. This framework is powered by the calculation of a Variance Reduction Potential (VRP) for each system inputs that relates how much how uncertainty in the system-level outputs are related to the uncertainty in the system inputs. This variance reduction potential can be estimated by simulating the system of interest. This allows for researchers to determine which variables are the most important to test before any testing has actually been done. This framework empowers researchers to gain as much information on their system as possible before spending resources on physical testing rounds, making research and development of new systems more efficient.

I. Nomenclature

Ε	=	Young's Modulus
G	=	Shear Modulus
МСМС	=	Markov Chain Monte Carlo
TRL	=	Technology Readiness Level
θ	=	Probabilistic System Input Parameter
UQ	=	Uncertainty Quantification
VRP	=	Variance Reduction Potential
v	=	Probabilistic System Output Parameter

II. Introduction

The task of developing a new technology to the point where it can be confidently integrated into a system design is a difficult problem that generally results in a complex, non-linear process that varies between organizations. The primary underlying concern in this task is the quantification and reduction of uncertainties in the technology, but this is often addressed with indirect methods that obfuscate this driving factor. There are many types of uncertainty that impact the confidence level of how well a technology might perform in a given system. This project focuses on epistemic, or reducible, uncertainty, which refers to a quality of the system that can be known given more information. This type of uncertainty is plentiful early in design or development processes when little is known about a system or technology. Even once a technology is matured enough to be applied to a specific system, its performance may differ greatly for an alternative system or use case which can require extensive work to re-qualify the technology.

Due to the complexity of the problem, it is difficult to determine the development progress for a technology in a general sense. This leads to projections and generalities such as readiness levels, which will be described in more detail below. Qualitative metrics such as these help to facilitate discussion between technology developers and potential users,

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but they are subject to irregularities since they are often based on generic milestones instead of quantifiable metrics of improvement. This work seeks to instantiate a framework to provide a more methodical and transparent process for assessing the progress of technology development through uncertainty quantification techniques, identifying key sources of uncertainty, assessing the impact of these uncertainty sources, and providing insight for how to systematically reduce uncertainties. These methods and tools will be developed, tested, and demonstrated on parametric finite element models, representing the implementation of a notional novel material technology in a system.

III. Background

In order to better understand this problem, multiple topics have to be addressed. These relate to the way that maturation is typically and generally defined, as well as the methods and tools related to the new approach proposed by the framework.

A. Technology Readiness Levels

A common method of relating the status of a technology is the Technology Readiness Level (TRL) scale, which is a single digit scale from one through nine developed internally at NASA and initially published in a 1989 white paper before going several rounds of revisions[1][2]. The terms readiness and maturity are sometimes used interchangeably, but in this context we will define maturity as the general feasibility of a technology and the readiness as the feasibility of a technology with respect to a specific system of interest. Therefore maturity of a technology will be system-independent and singular while it may have different levels of readiness for different systems. Many different types of readiness levels have been proposed such as Manufacturing, Integration, and Software readiness levels among others[3][4][5]. These scales have been proposed to supplement TRL or redefine the scale definitions to suit particular use cases. This work will focus on TRL to describe the overarching family of techniques.

Assessing the appropriate TRL for a technology in regards to a specified system is a non-trivial task. The definitions for each TRL for a technology are primarily based on which benchmark demonstrations the technology has successfully completed. The two primary methods of determining TRL are structured assessments such as those published by Mankins that rely on subject matter expertise, and detailed TRL calculators such as those published by NASA and the Air Force Research Lab that specify the full breadth of demonstrations that must be satisfied for a given readiness level [6]. Some combination of these demonstrations and subject matter expert opinions are used to generate a TRL for the technology.

However, there are limitations to these mostly qualitative processes. The activity of performing an experiment or demonstration would logically suggest that the level of knowledge about a technology has increased, which should thereby increase the TRL. However, the current a priori determination of benchmark experiments could potentially lead to conducting experiments that do not suitably address the currently problematic areas of uncertainty. The experimental results may simply validate something that was already assumed, and alternatively, performing the experiment does not guarantee that the resulting data was examined in a way which best benefits decision-makers. The synthesis of all the information regarding the status of a technology into a single value makes the TRL scale a valuable tool for high-level decision making. However, its basis on nominal benchmarks or subjective opinion can potentially lead to a lack of traceability and limits its ability to fully characterize the technology.

The TRL scale can be viewed effectively as an implicit encapsulation of the uncertainty in a technology. Shifting the technology development process to be based on uncertainty will create the information necessary for TRL to be explicitly based on specific categories and levels of uncertainty present in a technology at a given moment. The practical usability of the ordinal TRL scale succinctly summarizing the status of a technology cannot be ignored, so the aim of this work is to supplement its definitions with actionable and traceable information.

B. Bayesian Approach to Uncertainty Quantification (UQ)

The field of uncertainty quantification is a broad area, but generally involves creation of a distribution or similar measure to represent variation in a system attribute. This measure is then updated as more knowledge is generated with the goal of reducing the uncertainty of the parameter value. The initial creation of the distribution can come from expert elicitation [7] or data, be it collected from modeling and simulation or real world sources. As more data is generated, these initial distributions, called priors, are updated and refined into posteriors, representing the current understanding of variation.

There are two main schools of probability theory: objective (Frequentist) and subjective (Bayesian). The main



Fig. 1 Uncertainty Quantification Cycle

difference of these schools is that objective statisticians limit probability to only be meaningful over a long-run frequency, so uncertainty can only be relevant as the limit in the long run. Subjective statisticians can operate on subjective uncertainty with statistical and probabilistic tools, and this allows them to take a narrower view of uncertainty and apply them to single instances [8]. The introduction of subjective uncertainty in Bayesian statistics is incredibly powerful. It allows researchers to directly quantify their uncertainty in their knowledge of a system and compare it to test data. Then, as more data is generated about the system, researchers can directly quantify how this new data contributes to their existing knowledge.

As introduced above, there are two main types of uncertainty: aleatory and epistemic [9]. However, the sources of these uncertainties are vast and difficult to enumerate. Early in the quantification process, a variety of aleatory and epistemic uncertainties will all be aliased with one another, but gradually the sources should become less abstract. As previously discussed, the process of technology maturation is focused on identifying and reducing epistemic uncertainties so that the projected implications of application of a technology can be verified and validated to convince a system developer of its value. As more experiments are performed and models executed, the understanding of the system should improve. However, within this iterative process, there is a trade off between the attempt to quantify uncertainty without inserting additional or erroneous characteristics. To put it differently, the process of gathering data does not inherently beget lower uncertainty.

IV. Framework

The uncertainty quantification framework developed for this paper can be seen in Figure 1. As with any UQ process, it is iterative and consists of data gathering, data processing, and decision-making steps. These decision-making steps may be used in the future to determine whether a technology has advanced to the point where its level should increase, but those thresholds may be case specific and lie outside the scope of this work. It should be reiterated that in addition to the central goal of identification, quantification, and reduction of uncertainty, performing these steps include methods and tools that provide a greater understanding of the models, experiments, and system itself. One such secondary benefit is an improved capability to troubleshoot, debug, verify, and validate numerical models due to the insights gained about the relative relationships between inputs and responses.

A. Determination of Priors

In lieu of model or experimental data, early in the process, prior distributions must be estimated more from expert elicitation. Due to the semi-qualitative nature of such a step, one must seek to provide a justifiable starting point without over-determining variability. This leads to the discussion of "informativeness" of priors, which is related to the concentration of probability in a given dimension.

When the probability is more spread out, the prior can be referred to as diffuse, where a more informative prior will have a narrower range. Further confusing the issue, this classification as diffuse, weakly informative, or informative is situational. Additionally, even a diffuse prior can constrain the posterior distribution to a known region. A uniform distribution is an example of a diffuse prior, since it is simply dependent on an upper and lower bound [10].

B. Sampling

When attempting to populate a continuous distribution from discrete samples, a sampling method is needed. The most rudimentary sampling technique is a simple Monte Carlo, randomly selecting points within the variable space. However, it is well known that this method can be inefficient [11]. Despite that, due to the intended generality of the framework herein, and the emphasis on leveraging modeling and simulation to supplement physical experimentation, it can serve as the default approach. If it is known that the data generation source is inordinately expensive, a more efficient avenue can be employed, but that will be left up to the user for the time being.

C. Identifying and Selecting Critical Uncertainty Sources

The next step after prior determination in the UQ framework is the identification and selection of critical uncertainty sources, as seen in Figure 1. Critical uncertainty sources are parameters in the system of interest that have the most inherent uncertainty, and this uncertainty propagates up to the system-level outputs. In many cases, these parameters are determined using a main effects test like ANOVA. These tests highlight the parameters to which the output is the most sensitive. This can lead to an erroneous determination, though, because prior knowledge about the parameters is not taken into account. Therefore, this method can highlight a parameter as critical even though much is known about that parameters compared to other parameters. This may cause researchers to prioritize their efforts in areas that they have an abundance of knowledge in and ignore other areas that may yield more benefits in the context of system-level uncertainty reduction.

In an effort to incorporate prior knowledge into critical parameter identification, the authors of this paper have developed a metric they have named the Variance Reduction Potential. Say a system level metric y depends on a parameter θ . The posterior variance of the parameter θ for a given realization of y can be calculated using Equation 1 [12].

$$E(var(\theta|y)) = var(\theta) - var(E(\theta|y)) = var(\theta) \left(1 - \frac{var(E(\theta|y))}{var(\theta)}\right)$$
(1)

$$VRP = \frac{var(E(\theta|y))}{var(\theta)}$$
(2)

With this equation, the posterior variance of the parameter θ is inversely related to $var(E(\theta|y))/var(\theta)$, otherwise known as the Variance Reduction Potential, shown in Equation 2. Another way of framing this relationship is that the parameter θ is expected to reduce its variance proportional to the VRP after it has been conditioned the system level distribution of distribution of y. Therefore, the variances of the two parameters θ and y are linked through the VRP, and reducing the uncertainty of system input parameters with high values of VRP will reduce the uncertainty in the system-level outputs.

The Variance Reduction Potential can be estimated with computational simulation. This is done by simulating a large set of potential realized distributions and conditioning theta onto them using Bayes' Theorem (3) [12]. In order to develop the set of potential realized distributions, a simulator of the system must be available. This can be as complex as a detailed finite element model or a surrogate model, but it is recommended by the authors that the model complexity is as low as possible in order to be able to execute the model many times in a row. Then, using the prior distribution of the system parameters, many different potential values for the mean and variance of each system parameter are developed. Then, using these parameters to develop a distribution of the system output $(p(y|\theta))$. Then, a Markov Chain Monte



Fig. 2 VRP Estimation Process

Carlo (MCMC) method can be used to calculate the posterior distributions $(p(\theta|y))$ [13]. The authors of this paper used the Python package PyMC3 to implement the MCMC chains used in this work [14].

The distributions of these potential realizations of y are dependent on the system of interest. Once all of the conditioned posteriors of θ have been found, the VRP is estimated by calculating the variance of the posterior means of θ and normalizing it by the prior variance of θ , as seen in Equation 2. This normalization process makes the VRP vary from 0 to 1, thus making the VRP of different parameters directly comparable. This process is visualized in Figure 2.

$$P(\theta|y) = \frac{P(y|\theta)P(\theta)}{P(y)}$$
(3)

Once the VRP has been found for all of the parameters of interest, they are ranked by their magnitude. The parameter with the highest VRP is then chosen as the parameter with the most Variance Reduction Potential. This parameter should be selected as the most critical uncertainty source.

D. Reducing Uncertainty

Once the critical uncertainty source has been found, its uncertainty must be reduced. This is done through experimentation. The experiment or experiments that are selected are application dependent, but cost, time, fidelity, etc. should be considered when selecting the experiments to conduct. Once the experiments have been conducted, the distribution of θ should be recalculated. This should be done using Bayes' Theorem (3) where $p(\theta)$ is the previous distribution, $p(y|\theta)$ is the likelihood of the test data, and $p(\theta|y)$ is the posterior distribution of θ conditioned on the new test data. The posterior distribution will be the new prior distribution of θ in the next iterations of the cycle. A Bayesian statistics library like PyMC3 [14] can be used to determine the posterior distribution since p(y) is often difficult to calculate.

E. Propagate Uncertainty to the System Level

With the new priors for θ , computational modeling should be used to propagate this uncertainty up to the system level to get new distributions of the system level parameters. This can be done by conducting a Monte Carlo simulation of the system with the new posterior distribution of θ . Then, the distributions of the system outputs can be investigated to see the effect of reducing the uncertainty on θ to the system-level outputs.

V. Use Case

The framework described in this paper has been applied to a simple short cantilever beam model with an applied tip load, as shown in Figure 3. The output of interest in this model is the tip displacement. This model was chosen partly because it is known that the Young's Modulus has the most impact on the tip displacement, followed by a slight impact from the Shear Modulus. Additionally, this simple modeling framework has been parameterized for a number of material and geometry inputs and multiple corresponding model outputs for a previous work [15].



Fig. 3 Cantilever Beam Model

A. VRP Comparison for Different Priors

The framework described in this paper is able to determine the optimal system parameter to investigate based on the information already available to the experimenters. To study the effectiveness of the framework, a study based on different priors of the Young's Modulus and the Shear Modulus has been conducted. In this section, the uniform distribution will be denoted as U(L, H) where L is the lower bound and H is the upper bound of the distribution. The results of all of the VRP estimation cases can be seen in Figure 4.

1. ANOVA Results

For the model used in this paper, an ANOVA test was conducted to determine the relative importance of the Young's Modulus and the Shear Modulus. The model was simulated 1,000 times using random samples that were contained in E = U(9.86e6, 11.9e6) psi and G = U(3.6e6, 4.23e6) psi. Then, JMP[®] [16] was used to determine the log-worth of each parameter using $LogWorth = -log_{10}(p)$ where p is the p-value of each parameter. The results of this test were E has a log-worth of 551.3, and G has a log-worth of 121.9. This means that the Young's Modulus has a much greater impact on the tip displacement of the beam than the Shear Modulus.

2. Nominal Priors (Case1)

The nominal priors for the Young's Modulus and the Shear Modulus are E = U(9.86e6, 11.9e6) psi and G = U(3.6e6, 4.23e6) psi respectively. By applying the Variance Reduction Potential formula found in Section IV.C, the VRP of E and G are 0.29 and 0.0007 respectively. This indicates that E is the critical source of uncertainty with the nominal priors.

3. Lower Prior Uncertainty on E (Case 2)

In this section, assume that the experimenters have a large amount of prior information on the distribution of the Young's Modulus. The new distribution of the Young's Modulus is now assumed to be E = U(9.86e6, 9.9e6) psi. Now, applying the Variance Reduction Potential framework yields a VRP of 0.00014 and 0.00010 for E and G respectively. Now, E and G are essentially equal in terms of critical uncertainty. This demonstrates how infusing prior knowledge into the critical parameter determination can affect the results of the decision making process.

4. Higher Prior Uncertainty on G (Case 3)

In this section, assume that the experimenters have very little prior information on the distribution of the Shear Modulus. The new distribution of the Shear Modulus is now assumed to be G = U(3.6e6, 5.0e6) psi. With this new prior, the VRP of E and G are 0.40 and 0.006 respectively. This is an interesting result, because it indicates that E is



Fig. 4 Results of the VRP Estimation Cases

more critical to reduce than G even though the uncertainty for G has increased. The framework has determined that reducing the uncertainty in the Young's Modulus can compensate for the increased uncertainty in the Shear Modulus.

5. Lower Prior Uncertainty on E and Higher Prior Uncertainty on G (Case 4)

In this section, assume that the experimenters have little prior information on the distribution of the Shear Modulus and a large amount of information on the distribution of the Young's Modulus. The new distribution of the Shear Modulus is now assumed to be G = U(3.6e6, 5.0e6) psi, and the new distribution of the Young's Modulus is now assumed to be E = U(9.86e6, 9.9e6) psi. With these new priors, the VRP of E and G are 0.00014 and 0.00015 respectively. This result further solidifies the conclusion found in case 3. While the researchers have a lower understanding of the Shear Modulus in this case than in the nominal case, the VRP of the Shear Modulus is still very low and on the same magnitude as the Young's Modulus. This is because the researchers have a higher understanding of the Young's Modulus in this case than in the nominal case. This demonstrates that the Young's Modulus is much more important to the system behavior than the Shear Modulus, and therefore it is extremely important to generate test data for the Young's Modulus.

VI. Conclusions

In this work, a framework is developed to use uncertainty quantification to help technology evaluators find and drive down the main sources of epistemic uncertainty. This process is demonstrated using a notional new material system applied to a parametric finite element model of a beam. Priors are generated, propagated through the modeling environment, and analyzed to help quantify and justify potential future work that can help with the adoption of a technology. Future work can include evaluation of more advanced sampling techniques when evaluations are more expensive, as well as expansion in the decision-making capabilities to provide an even deeper understanding for the technology developer and to help further define the rate of maturity.

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