A value-of-information based approach to simulation model refinement

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The appropriateness of a simulation model for engineering design is dependent on the trade-off between model accuracy and the computational expense for its development and execution. Since no simulation model is perfect, any simulation model for a system’s physical behaviour can be refined further, although likely at an increased computational cost. Hence, the question faced by a designer is – “How much refinement of a simulation model is appropriate for a particular design problem?” The simplified nature of simulation models results in two types of uncertainty: a) variability, that can be modelled using probability distribution functions and b) imprecision, that is best modelled using intervals. Value-of-information has been used in the engineering design literature to decide whether to make a decision using the available information or to gather more information before making a decision. However, the main drawback of applying existing value-of-information based metrics for model refinement problems is that existing metrics only account for variability; they do not account for imprecision in simulation models and the impact of its reduction on design decisions.

To overcome the limitation of existing metrics in the context of model refinement, we present a value-of-information based approach for determining the appropriate extent of refinement of simulation models. The approach consists of i) a metric called improvement potential for quantifying the value of information obtained via refinement of simulation models and ii) a method in which this metric is utilized for supporting model refinement decisions. The improvement potential measures the value of information by considering both imprecision and variability in simplified models. It quantifies the maximum possible improvement in a designer’s decision that can be achieved by refining a simulation model. Specifically, we focus on multi-objective compromise decisions modelled using the compromise Decision Support Problem construct, which is a hybrid formulation based on traditional optimization and goal programming. The method involves starting from a simple simulation model and gradually refining it until the value of further refinement on design decisions is small. The approach is presented using two examples – design of a pressure vessel and design of a multifunctional material. The pressure vessel problem is used to illustrate the benefits of using this approach are shown by gradually refining its material parameters; the materials design problem is a comprehensive problem where a complex finite element model is gradually refined. The approach proposed in this paper can be utilized by designers and analysts in developing effective simulation models for specific design problems while efficiently utilizing their model development resources.

Keywords: Simulation models; refinement; value of information; decision making

GLOSSARY

Model refinement: Improving the fidelity of a simulation model to improve a designer’s decision making ability.

Value of information from model refinement: An increase in the overall utility value when a refined model is used as compared to the original model.

Improvement Potential: The maximum possible improvement in a designer’s decision that can be achieved by refining a simulation model. It is measured as the upper-bound on the increase in expected utility through model refinement.

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1 In this paper, we assume that the decision maker uses utility functions to quantify the payoffs. Hence, the word ‘payoff’ is used synonymously with ‘utility’ in the rest of the paper.
### Nomenclature

(in the order of appearance)

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H$</td>
<td>Hurwicz Utility</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Coefficient of pessimism, measuring decision maker’s aversion to risk</td>
</tr>
<tr>
<td>$U_{\text{min}}$</td>
<td>Lower bound on expected utility</td>
</tr>
<tr>
<td>$U_{\text{max}}$</td>
<td>Upper bound on expected utility</td>
</tr>
<tr>
<td>$\pi$</td>
<td>Payoff bound</td>
</tr>
<tr>
<td>$v$</td>
<td>Value of a decision</td>
</tr>
<tr>
<td>$X_1$</td>
<td>Decision made using the actual system behavior</td>
</tr>
<tr>
<td>$X_2$</td>
<td>Decision made using predicted system behavior</td>
</tr>
<tr>
<td>$U_1$</td>
<td>Payoff (utility) achieved if the actual system behavior is used for decision making</td>
</tr>
<tr>
<td>$U_2$</td>
<td>Payoff (utility) achieved if the predicted system behavior is used</td>
</tr>
<tr>
<td>$P_I$</td>
<td>Improvement potential</td>
</tr>
<tr>
<td>$(U_{\text{min}})^*$</td>
<td>Lower bound on expected payoff at decision point</td>
</tr>
<tr>
<td>$(U_{\text{max}})^*$</td>
<td>Upper bound on expected payoff at decision point</td>
</tr>
<tr>
<td>$\max(U_{\text{max}})$</td>
<td>Maximum of upper bound on utility throughout the design space</td>
</tr>
<tr>
<td>$H^*$</td>
<td>Hurwicz utility at decision point</td>
</tr>
<tr>
<td>$S_t$</td>
<td>Strength of the material used for the pressure vessel</td>
</tr>
<tr>
<td>$P$</td>
<td>Maximum pressure in the pressure vessel</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density of the material used for pressure vessel</td>
</tr>
<tr>
<td>$L$</td>
<td>Length of the pressure vessel</td>
</tr>
<tr>
<td>$R$</td>
<td>Radius of pressure vessel</td>
</tr>
<tr>
<td>$T$</td>
<td>Thickness of the plate used to manufacture the pressure vessel</td>
</tr>
<tr>
<td>$V$</td>
<td>Volume of the pressure vessel</td>
</tr>
<tr>
<td>$W$</td>
<td>Weight of the pressure vessel</td>
</tr>
<tr>
<td>$U_W$</td>
<td>Utility for the weight goal</td>
</tr>
<tr>
<td>$U_V$</td>
<td>Utility for the volume goal</td>
</tr>
<tr>
<td>$U_{\text{overall}}$</td>
<td>Overall utility – calculate by combining the individual utilities</td>
</tr>
<tr>
<td>$Z$</td>
<td>Deviation function</td>
</tr>
<tr>
<td>$V_p$</td>
<td>Particle velocity in the materials design problem</td>
</tr>
<tr>
<td>$V_s$</td>
<td>Shock speed in the materials design problem</td>
</tr>
<tr>
<td>$R_{\text{Al}}$</td>
<td>Radius of Aluminum particles in the materials design problem</td>
</tr>
<tr>
<td>$VF_{\text{Voids}}$</td>
<td>Volume fraction of voids in the material</td>
</tr>
<tr>
<td>$S_C$</td>
<td>Size of the cells in the shock simulation model</td>
</tr>
<tr>
<td>$S_w$</td>
<td>Window size in the shock simulation model</td>
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1. Frame of Reference – Simulation Model Refinement

Design is a decision-making process involving the transformation of a product’s functional requirements into its structure (Mistree et al. 1990, Muster and Mistree 1988). Design decisions are generally made based on the information about the products’ performance as a function of its structure. This information can be obtained through physical testing, previous experience, or simulation models. Simulation-based design is a field in engineering design where the focus is on using simulation models for making design decisions. In the past few decades, significant efforts have focused on a) developing accurate simulation models for complex systems, and b) high performance computing to support these complex models. In spite of the significant progress in both these areas, modelling all aspects of a complex system in a simulation model is not possible using the currently available computational resources. This is further emphasized by a quote by George Box: “All models are wrong, some models are useful” (Box 1979). According to this statement, all models have some approximations and they can be refined through various means. Some means for refinement of simulation models include the consideration of additional physical phenomena and their interactions in the model, finer grids in Finite Element based models, or better estimation of experimental parameters used in the model.

Refinement of a simulation model improves its accuracy but also increases the associated costs for both modelling and execution. We believe that the role of simulation models in engineering design is not to predict the behaviour of a system exactly, but to support design decisions. Despite the fact that the accuracy of simulation models influences the quality of design decisions, designers do not need (and cannot have) perfect models for making design decisions. A simulation model is good in the context of design if it helps designers make good design decisions. Although simulation models can be refined indefinitely, after a certain level of refinement of simulation models, simplified models can be used to make “satisficing” (good enough) decisions (Simon 1996). In this context, the question that a designer faces is: How much refinement of a simulation model is appropriate for a particular design problem?

Radhakrishnan and McAdams (Radhakrishnan and McAdams 2005) address a similar problem of model selection in engineering design using a utility based approach. They formulate preferences for accuracy in the model, and the costs incurred in constructing the model. The model with the maximum expected utility is selected. The core assumption in their approach is that all the model options are available along with the information about their accuracy and cost. In the case of the model refinement problem, however, this information is not available. Designers start with a simple model and systematically refine it until a model that is good enough for decision making is obtained. Further, the authors do not consider the impact of model selection on the design decisions. We believe that the refinement of a simulation model should not only be based on its accuracy, but also on the outcome of decisions made using the model (Ling 2006, Panchal 2005).

In this paper, we present a value-of-information based approach for systematic refinement of simulation models from the standpoint of multi-objective design decision-making. These decisions are modelled using the compromise Decision Support Problem (Mistree et al. 1993, Seepersad 2001) construct, which is a hybrid formulation based on mathematical programming and goal programming. The approach for model refinement consists of a value-of-information based metric to quantify the improvement in decision making from refining the simulation model, and method for stepwise model refinement. In the context of simulation-based design, a simulation model is a source of information. Refining a simulation model is equivalent to adding more information for decision making so that the model more accurately predicts the behaviour of the system. The metric presented in this paper is called the Improvement Potential. It quantifies the maximum possible improvement in a designer’s decision (in terms of utility) that can be achieved by refining a simulation model. For a given model, the improvement potential is evaluated. If the potential is high, the model is refined further otherwise it is used for making design decision. The refinement is carried out in a stepwise manner, with
improvement potential calculated at each step, until the model is appropriate for the design decision. Using this approach, designers and analysts can develop effective simulation models for specific design problems in a resource efficient manner.

The paper is organized as follows. Related literature and background on decision making and value of information is provided in Section 2. The approach proposed for simulation model refinement is presented in Section 3. Two examples - design of pressure vessels and design of materials - are presented in Sections 4 and 5 to illustrate the use of the approach. The pressure vessel design problem is used as an illustrative example to show the benefits of using value of information in making refinement decisions. In this problem, the refinement is achieved by simply reducing the bounds on parameters. On the other hand, the materials design example represents a typical problem encountered in simulation-based design where the refinement of a Finite Element model is carried out by increasing the size of the domain modelled, and refining the Finite Element mesh. Finally, closing thoughts are presented in Section 6.

2. Background – Decision making Under Uncertainty and Value of information

In this section, we discuss different types of metrics for value of information (Section 2.2) and the application of value of information concepts in design decision making (Section 2.3). Existing research efforts on applying value of information concepts in design are discussed in Section 2.3.1, and the limitations of existing efforts are discussed in Section 2.3.2. In order to provide a background for the existing efforts, we first present an overview of decision making under different types of uncertainty (Section 2.1).

2.1 Decision Making under Different Types of Uncertainty

Uncertainty in simulation models is broadly classified into two types – variability and imprecision. Variability is the type of uncertainty that is inherent in the system being modelled and is represented using probability distributions. It is also referred to as stochastic uncertainty. In contrast to variability, imprecision is generally modelled using intervals (Moore 1966, Ward et al. 1990) or fuzzy sets (Antonsson 2001, Antonsson and Otto 1995, Wood and Antonsson 1989). Antonsson and Otto define an imprecise variable as “a variable that may potentially assume any value within the possible range” (Antonsson and Otto 1995). Fuzzy sets are used to model a designer’s preference for specific values of design parameters in addition to the imprecision in the design variables. The key difference between imprecision and variability is that imprecision is a type of epistemic uncertainty (i.e., the lack of knowledge), whereas variability is a type of aleatory uncertainty (i.e., inherent randomness in the system). From a value-of-information standpoint, imprecision can be reduced by incorporating more knowledge via refinement of simulation models but the variability that is inherent in the system behaviour cannot be reduced by gathering more information.

Decision making under variability and imprecision in simulation models is illustrated separately in Figure 1(a) and Figure 1(b), respectively. Consider the scenario shown in Figure 1(a), where a designer needs to select between two design alternatives A and B. Due to the system variability, the uncertain payoff values for both these alternatives are best represented as probability distributions. The decision criterion in such a scenario is to select the alternative that results in maximum expected payoff when taking risk attitudes into account (Keeney and Raiffa 1976). In this paper, we use utility functions to measure the payoff. Utility functions are used to quantify a designer’s preferences for outcomes achieved for different alternatives (Von Neumann and Morgenstern 1947). For simplicity, we assume that the utility of an ideal outcome is 1 and the utility of an unacceptable outcome is 0. The shape of a utility function represents a designer’s attitude towards risk; a convex utility function implies risk aversion whereas a concave utility function implies risk proneness. For details on the characteristics of utility functions, please refer to (Keeney and Raiffa 1976). According to utility theory, “if an appropriate utility is assigned to each possible outcome and the expected utility of the outcome
for each alternative is calculated, then the best course of action is to select the alternative whose outcome has the largest expected utility” (Keeney and Raiffa 1976). Hence in Figure 1(a), a designer would select alternative A because the expected utility (payoff) is greater than for alternative B.

An approach for selection of alternatives based on maximization of expected utility is presented by Fernández and co-authors (Fernández et al. 2005). The decision criterion of maximization of expected utility is extended to multi-objective decisions by Seepersad and co-authors (Seepersad 2001, Seepersad et al. 2005) in the Utility-based Compromise Decision Support Problem. In this formulation, individual goals are formulated as single attribute utility functions, and multiple goals are combined in the objective function using Archimedean weightings (Seepersad et al. 2005). The Utility based compromise DSP formulation is used in this paper to formulate multi-objective design decisions. The mathematical formulation is provided in Figure 2.

In the scenario shown in Figure 1(b) the payoffs for the Alternatives C and D are imprecise and are best represented by intervals. Since the representation is non-probabilistic, maximization of expected utility cannot be used as a decision criterion. In this scenario, one possible decision criterion is to select the alternative with the highest upper bound on payoff (maximax criterion). Such a criterion reflects a designer’s complete optimism. An alternative decision criterion involves selecting an alternative that maximizes the lower bound on payoff (maximin criterion), reflecting a designer’s complete pessimism. Using the maximax criterion, a designer would select Alternative C, whereas Alternative D is chosen when the maximin criterion is considered. Different decision criteria are appropriate in different design scenarios. A third type of decision criterion, called the Hurwicz criterion (Arrow and Hurwicz 1972), is based on the combination of optimistic and pessimistic criteria. The Hurwicz decision criterion involves maximizing a weighted average ($H$) of lower and upper bound.

$$H = (\alpha) \text{ (Lower Bound)} + (1-\alpha) \text{ (Upper Bound)}$$

The weighted average is calculated using a coefficient of pessimism ($\alpha$) that is a measure of a decision maker’s aversion to risk under imprecision. An $\alpha=1$ implies complete pessimism (maximin) and $\alpha=0$ implies complete optimism (maximax). Using a pessimism index of $\alpha=0.5$ in Figure 1, a designer would select alternative C.

In a design scenario, the model can have both statistical variability and imprecision. In such a scenario, the Hurwicz criterion can be applied on the intervals of expected payoff. For each alternative, the lower and upper bounds on expected payoff are determined. Using the pessimism index, a weighted average of expected utility is determined for each alternative. The alternative with maximum weighted average is selected. Throughout this paper, we use this decision criterion to select an alternative or a point in the design space. A pessimism index of $\alpha=0.5$ is used in this paper unless explicitly stated to be different.

### 2.2 Value of Information in Decision Making

At any stage in the decision making process, designers possess some amount of information that can be used for selecting the best course of action. Designers have an option of either i) making a decision using the available information, or ii) gathering more information and then making a decision using the updated information. In this context of decision making, the value of this added information refers to the improvement in a designer’s decision making ability. The refinement of simulation models is analogous to the acquisition of a new source of information, and the set of results from the execution of this refined model is analogous to additional information for decision making. Hence, value-of-information based metrics can be used by decision makers to make meta-level decisions involving a trade-off between reduced uncertainty and increased cost as a result of refinement of simulation models. The increase in cost is due to both refinement and execution of a more complex model.
Consider for example a designer who has a simulation model for predicting the system behaviour and is interested in making a decision using the model. Before making the decision, he/she has an option of increasing the fidelity of the model by including additional physical phenomena in the model. For example, a structural designer may improve the fidelity of a statics model by adding dynamic behaviour, or creep. Inclusion of a physical phenomenon in the simulation model is equivalent to an information source that generates information about the system behaviour. The output of the simulation (i.e., the predicted system behaviour) is equivalent to the added information generated by the information source.

Howard (Howard 1966) has proposed the use of value of information for determining whether to consider additional information for decision making. The expected value of information, as defined by Howard, is the difference between the expected value of the objective for the option selected with the benefit of the information less than without. Lawrence (Lawrence 1999) provides a comprehensive overview of metrics for value of information. He argues that the value of information for decision making can be measured at different stages in the decision making process: a) prior to consideration of incorporation of information, b) after considering a message source but prior to receiving a message (ex-ante value), c) after receiving additional information and making the decision, but before realization of the environmental state (conditional value), or d) after addition of information and observing the outcome of the decision based on acquired information (ex-post value). Referring back to the structural decision maker, the decision maker can evaluate the expected value of information before even considering the incorporation of any additional physical phenomena. The second option (ex-ante value) is to decide which physical phenomena to model (i.e., which information source to choose) and to evaluate the value of information before executing the simulation code. The third option (conditional value) is to evaluate the value after executing the simulation code and making decision about the system but before manufacturing and testing the system. The fourth option (ex-post value) is to evaluate the value of this additional information after making decisions and also manufacturing and testing the system.

Mathematically, the ex-ante and ex-post value-of-information based metrics are represented as follows:

\[
\text{Ex-ante value: } V(x, y) = E_{a_y} \pi(x, a_y) - E_x \pi(x, a_0)
\]

\[
\text{Ex-post value: } V(x, y) = \pi(x, a_y) - \pi(x, a_0)
\]

where \( E_x f(x) \) is the expected value of \( f(x) \) and \( E_{a_y} f(x) \) is the expected value of \( f(x) \) given \( y \). The symbols \( a_0 \) and \( a_y \) represent the actions taken by the decision maker in the absence and presence of information \( y \) and \( \pi(x, a) \) represents the payoff achieved by selecting an action \( a \), when the state realized by the environment after the decision is \( x \). It is important to realize that the key difference between ex-ante and ex-post value is that in ex-post value, the realization of the state \( x \) is known. However, the realization of the state \( x \) is not known in the ex-ante value and the expected value of payoff is taken over the uncertain range of state \( x \).

Ideally, designers prefer the ex-post value-of-information because it truly reflects the value of information for a decision based on the actual behaviour of the system. At that stage, the realization of the state \( x \) is known and the system behaviour can be measured exactly. However, it is not possible to predict the ex-post value of a decision before making the decision itself. Due to the ex-ante nature of decision making, the decisions about the information have to be made before the state actually occurs. Hence, the designers are left with using ex-ante value-of-information. It captures the value-of-information by considering uncertainties in the system.
2.3 Value of Information Metric to Support Design Decisions

2.3.1 Existing Research Efforts on Value of Information
A summary of the existing efforts on applying value of information in engineering is provided in Table 1. In the context of engineering design, Agogino and co-authors (Agogino 1997, Bradley and Agogino 1994, Bradley et al. 1994, Wood and Agogino 2005) present a metric called the Expected Value of Information (EVI) and use it for a catalog selection problem (Bradley and Agogino 1994), where a designer is faced with the task of choosing components from a catalog in order to satisfy some functional requirements. During the conceptual design phase, selection decisions need to be made under significant uncertainty, for example, due to a limited understanding of requirements and constraints, an inability to specify part dimensions, or uncertainty in the environmental conditions. Before making the decision about selecting the right component, a designer is faced with another higher level decision – whether to go ahead and make the decision using the available information or to spend resources and gather more information before making the selection decision. This is a process-level decision, for which Bradley and Agogino (Bradley and Agogino 1994) use EVI to quantify the expected benefit from additional information. The EVI is equal to the expectation of objective function over the uncertain variables with new information minus the expectation of the objective function with current state of information. Evaluation of the EVI requires the availability of probability distributions over uncertain variables with new information, which is not available before the refinement of the simulation model. Hence, the EVI is not suitable for model refinement decisions. Further, the focus of research by Agogino and co-authors is on the refinement of information about design concepts and the evaluation function in the conceptual design phase (Pahl and Beitz 1996) whereas our focus in this paper is on refinement of simulation models to be used in the embodiment design phase (Pahl and Beitz 1996).

Poh and Horvitz (Poh and Horvitz 1993) use a value-of-information metric for refining decisions. The authors present three dimensions in which decisions can be refined – quantitative, conceptual, and structural. Quantitative refinement of a decision can be carried out by reducing the uncertainty in the decision problem or by refining the preference models. Conceptual refinement is carried out by refining the definition of alternatives and design variables, whereas structural refinement requires addition of dependencies in the simulation model. Poh and Horvitz use the value-of-information metric to determine which dimension is critical for refinement of the decision problem.

In order to model variability for evaluating value of information, it is generally assumed that the probability distributions are available. However, if these probability distributions are not available, they are generally generated through an educated guess that is based on a designer’s prior knowledge. In order to address the problem of lack of knowledge about the probability distributions, Augenbaugh and co-authors (Augenbaugh et al. 2005) present an approach of measuring the value of information based on probability bounds. They assume that although the exact probability distributions are unavailable, the lower and upper bounds on these probability distributions are available in terms of p-boxes (Ferson and Donald 1998). Using this p-box approach, they evaluate the value of added information that reduces the size of the interval for probability distributions (i.e., tightens the probability bounds).

2.3.2 Limitations of Existing Approaches in the Context of Simulation Model Refinement
In previous research efforts by Howard (Howard 1966), Agogino & co-authors (Bradley and Agogino 1994), and Lawrence (Lawrence 1999) the value of information is calculated by considering only the stochastic variability, where the decision can be made by maximizing the expected value of the objective function. These efforts do not address the case of decision making under imprecise information (see Table 1). For example, consider a scenario where a designer has an option of making a decision using one out of two available simulation models. One of the simulation models has a higher fidelity representation of physics than
the other. The difference in the results simulation models is best represented as imprecision rather than statistical variability. Such a scenario is extremely common in multi-scale design problems. The consideration of imprecision while measuring the value of information in addition to variability is very important from the standpoint of simulation model refinement. It forms a basis for determining the extent of refinement of simulation models. Hence, the primary need for a new value-of-information based metric for model refinement is quantification of the impact of imprecision in simulation models. Except for Aughenbaugh and co-authors (Aughenbaugh et al. 2005), imprecision in data, which cannot be modelled in terms of probability distribution functions is often not modelled at all in the existing efforts. Aughenbaugh and co-authors (Aughenbaugh et al. 2005) focus on modelling the effect of imprecision in probability distribution functions on data collected from physical experiments whereas in this paper, we focus on modelling the imprecision in the outputs parameters of simulation models and the effect of reducing this imprecision by refining the models. As a summary, the primary limitation of the existing value of information metrics for model refinement is that existing metrics do not account for imprecision in simulation models and the impact of reduction of imprecision on design decisions. In this paper, we address this limitation by proposing a metric that accounts for both imprecision and variability in simulation models.

3. Value-Based Approach for Simulation Model Refinement

3.1 Value-Of-Information Metric for Model Refinement

3.1.1 Measuring the Value of a Perfect Model
Consider a scenario shown in Figure 3, where the horizontal axis is the value of the design variable and the vertical axis is the corresponding payoff that is achieved by selecting the design variable. The design variable can be some physical dimension that a designer has control over, whereas the payoff represents profit, which depends on system behaviour such as performance, strength, and cost. A designer’s objective is to maximize the expected payoff through selection of an appropriate design variable value. The solid line represents the expected payoff evaluated using actual system behaviour and the dashed line represents the payoff evaluated from system behaviour predicted by the simulation model. The difference in actual and predicted behaviour corresponds to the imprecision and is due to simplifications in the model. In this scenario, the statistical variability is accounted for by taking the expected payoff. The focus of refinement in this paper is only on reducing the imprecision resulting from the simplified nature of simulation models.

If a designer makes a decision using the simulation model only, the decision point is \( X_2 \), because it maximizes the expected payoff based on the predicted behaviour. By selecting the decision point \( X_2 \), the designer would actually achieve the payoff equal to \( U_2 \) because the system’s actual behaviour is given by the solid line. However, a designer would have selected decision point \( X_1 \) if the actual (real) behaviour of the system were known (by using a perfect model). For the decision point \( X_1 \), the actual payoff achieved is the maximum (\( =U_1 \)). Hence, the value of using the perfect model over the simpler model is the difference in expected payoff actually achieved. It is important to note that the value of information is evaluated by measuring the difference in payoff using the actual system behaviour \( (U_1-U_2) \). It can only be evaluated if a) the actual system behaviour is known or b) it is calculated after the decision is made and the outcome is realized. Hence, this value-of-information metric is similar to the ex-post value used in the literature.

Notice that the value of information as shown in this figure captures the benefit (the improvement in expected payoff) of using the actual system behaviour over the predicted system behaviour from the simplified model. Hence, it refers to the value of perfect information. As mentioned in Section 2.1, the payoff is quantified using utility functions whose lower and upper bounds are 0 and 1 respectively. Since the value of perfect
information is measured as a difference between two utility functions, it also lies between 0 and 1. It is zero if the decision made using the simulation model is the same as the decision made using the actual system behaviour (i.e., $X_1 = X_2$). This scenario is shown in Figure 4(a). If this value of perfect information is zero, the benefit from using the actual system behaviour over the predicted behaviour is zero. This implies that the simulation model is perfect for decision making. On the contrary, if the value of perfect information is high, one should consider refining the simulation model. In other words, this metric quantifies the value of refining the simulation model. The worst case scenario, shown in Figure 4(b), occurs when the maximization of expected utility using the predicted model results in $U_2 = 0$, while the ideal maximum payoff $U_1 = 1$. In this scenario, the value of perfect information is equal to 1 (because $U_1 - U_2 = 1$). Further, the value of perfect information is always non-negative.

It is important to realize that the value does not depend on the accuracy of the model only. It also depends on the complete decision formulation that includes constraints, preferences, region in the design space that is under consideration, etc. This point is illustrated further in Section 4 using a design example. The same concept extends to higher dimensional problems where there are many design variables and the payoff is determined by multiple conflicting criteria. In the case of multiple design variables, the curve corresponds to a multidimensional surface. In the case of multiple design criteria that affect the payoff, the criteria are combined together into an overall payoff function based on designers’ preferences.

The value of perfect information can be augmented to measure the value of information from model refinement, which is the increase in the expected utility achieved when a refined model is used as compared to a simplified model. For calculating the value of perfect information (as shown conceptually in Figure 3) before making a decision, a designer needs to know the actual system behaviour. However, in most design cases, the difficulty is that the exact system behaviour is unknown. If the exact system behaviour were available, there would be no need to use the simulation model to predict the behaviour. Hence, the use of value of perfect information shown in Figure 3 is impractical in a real design scenario. To overcome this difficulty in practical use, a variation in the value of perfect information is presented next.

### 3.1.2 Measuring the Improvement Potential

Although the exact system behaviour is unknown in most design scenarios, in many cases it is possible to determine an upper and lower bound on the behaviour predicted by a simulation model. Designers may be able to generate information about lower and upper bounds through physical experiments, or through analysts’ insights into the system’s behaviour. These bounds on the imprecision of the model result in bounds on the overall utility function, as shown in Figure 5. In this figure, the lower and upper bounds on the utility function ($U_{\text{min}}$ and $U_{\text{max}}$ respectively) represent the range within which the expected utility calculated from actual system behaviour (i.e., the solid curve shown in Figure 3) lies. The value of information metric developed in this paper is based on the assumption that bounds on imprecision of simulation models are available.

With the available information about lower and upper bounds on payoff, the decision maker can select a decision rule based on which he/she selects numerical values for the design variables. As discussed earlier in this section, the decision rule can be a) maximize the lower bound on achievable payoff (i.e., the worst case scenario), b) maximize the upper bound on achievable payoff (i.e., best possible scenario), or c) maximize a weighted combination of payoff (Hurwicz criterion). For the selected value of the design variable, there is a range of achievable payoffs as a result of imprecision in the simulation model. The lower bound on expected payoff is denoted by $U_{\text{min}}$, the upper bound by $U_{\text{max}}$, and the payoff evaluated using Hurwicz criterion by $H$. The lower and upper bounds on expected payoff at the decision point are denoted as $(U_{\text{min}})^*$ and $(U_{\text{max}})^*$ respectively. The maximum payoff that can possibly be achieved by any value of the design space is $\max(U_{\text{max}})$, and is evaluated by maximizing the upper imprecision bound on payoff. Since the exact value of the payoff is not known at different values of design variables, it is not possible to calculate the exact value of information as illustrated in Figure 3. However, since the lower and upper bounds on payoff are known
throughout the design space, we can determine the maximum possible value of information. This upper bound on the value of information (maximum possible value) is referred to as the improvement potential ($P_I$) and is given by:

$$P_I = \max(U_{\text{max}}) - (U_{\text{min}})^*$$

where $\max(U_{\text{max}})$ is the maximum expected payoff that can be achieved by any point in the design space and $(U_{\text{min}})^*$ is the lowest expected payoff value achieved by the selected point in the design space (after making the decision without added information). We propose the improvement potential as a value-of-information metric for deciding whether further refinement in the simulation model is necessary or not. This metric is used in the method for stepwise refinement discussed in Section 3.2.

### 3.1.3 Properties of the Improvement Potential Metric

The first important property of the improvement potential metric discussed in Section 3.1.2 is that it also captures the effect of imprecision in simulation models in the evaluation of value of information. Statistical variability is accounted for by using the expected utility and imprecision is accounted for by using the lower and upper bounds on expected utility. Hence, it overcomes the limitations of existing metrics discussed in Section 2.3.2. Although the metric can be used in the cases where both imprecision and variability are present, in this paper we only focus on the imprecision in simulation models.

The second important property of the value-of-information metric is the ability to quantify the opportunity for improving the design solution by adding more information. That is, the proposed value-of-information metric quantifies the upper bound on the benefit that can be achieved by obtaining perfect information. The opportunity for improving the design solution is quantified in the literature using the Expected Value of Perfect Information (EVPI) (Bradley and Agogino 1994), which is calculated as the expected value of information based on setting the numerical values of uncertain parameters equal to their actual realization. If there are multiple uncertain parameters, the expected value of perfect information corresponding to each parameter is evaluated for individual parameters by setting their exact values. The greater the expected value of perfect information, the greater is the opportunity of improving the design solution through information gathering. The limitation of this EVPI, however is that the exact values of parameters are generally not available before gathering the information. In contrast, the advantage of the improvement potential is that it provides an indication of the opportunity without necessitating the perfect information.

### 3.1.4 Scope of the Proposed Metric for Simulation Model Refinement

The value-of-information metric presented in this paper is based on the assumption that information about error bounds (i.e., the lower and upper bounds on the imprecise variables) is available. The metric is not applicable if this information is not available. For example, if there are different fidelities of simulation models available but there is no information about the bounds within which the actual behaviour lies, then the metric cannot be used. The metric is ineffective if one of the bounds were incorrect (i.e., the real value lies outside the bounds). There is a need to develop new metrics that address such scenarios.

The metric is developed considering only the information about the improvement in payoff of the decision. It does not include the cost of gathering the additional information (the cost of reducing the range of imprecise variables in the case of simulation model refinement). It is assumed that for a given step in the series of refinement steps, a designer evaluates the estimated cost of gathering information and the value of this added information. Using these two indicators, a designer makes the decision on whether additional information is worth gaining. Strictly speaking, there is a trade-off between the improvement potential and the cost (of refining a simulation model and executing the refined model). In this paper, we limit the scope of the improvement potential to the benefit achieved by refining the simulation model. The cost of model refinement will be considered in a future publication.
Finally, the metric can only be used to determine whether a given level of refinement of simulation model is appropriate for making a particular decision or not and it is done after the computations have been made. It does not help designers in determining how much refinement is required in the simulation model.

### 3.2 Method for Stepwise Model Refinement using Value of Information

The method for stepwise refinement of simulation models is shown in Figure 6. The method consists of seven steps:

**Step 1:** The first step in this method is to formulate a design decision. The decision is formulated using a compromise DSP formulation. The mathematical formulation for a compromise DSP is given in Figure 2 and the mathematical decision formulations for the design problems are presented in Sections 4.1 and 5.2.1.

**Step 2:** In order to make this decision, a designer starts with a simple simulation model that is associated with imprecision in outputs. The strategy adopted in this method is to start with a simple model (that is computationally inexpensive) and to refine it gradually until it is appropriate for the decision. For each of the refined models being considered, the designer performs steps 3 through 7.

**Step 3:** Information about the lower and upper imprecision bounds on the output of a simulation model is gathered. Using this information, two optimization problems are solved in Steps 4 and 5, respectively.

**Step 4:** In this step, the first optimization problem is solved, in which the designer determines a point in the design space that maximizes the Hurwicz weighted average of expected utility ($H$). This point is called the decision point. The lower bound on the expected utility at this decision point is determined ($U_{\text{min}}^*$).

**Step 5:** In the second optimization problem, the designer determines $\max(U_{\text{max}})$, which is the maximum of the upper bound on the expected utility (maximax criterion).

**Step 6:** The improvement potential is determined using $p_I = \max(U_{\text{max}}) - (U_{\text{min}}^*)$.

**Step 7:** If the improvement potential evaluated in Step 6 is high (implying that gathering more information via model refinement is beneficial), the model is refined and an updated decision is made. The model is systematically refined in this manner until the value of additional information is low (i.e., the model is good enough for decision making). The magnitude of the improvement potential directly relates to the achievement of the designers’ goals. Hence, deciding whether the improvement potential is low enough depends on the design problem and the cost of improving the model to achieve that improvement. The relationship between the improvement potential and the design goals is elaborated using pressure vessel example in Section 4.2.1.

The approach discussed in this section is illustrated through two examples – design of a pressure vessel and the design of materials. The pressure vessel design problem is used as a simple illustrative example. Since the problem consists of only one design variable, the results can be easily plotted and insights can be gained by graphical means. The imprecision in this problem is due to the range of possible property values of the material used to manufacture the pressure vessel. The material design example is a comprehensive example where a Finite Element Model is used to predict the behaviour of a material by changing multiple design variables. The imprecision in this example is due to the small size of the domain considered, and the discretization errors. The materials design example represents a typical simulation-based design problem. The pressure vessel design example is discussed in Section 4 and the material design example is discussed in Section 5.
4. Example – Design of Pressure Vessel

4.1 Problem Description – Pressure Vessel Design

In this section, we discuss an example design problem where the objective is to design a pressure vessel with low weight and high volume. This problem is adapted from (Marston 2000), and more details about the example problem are available in (Panchal 2005). The pressure vessel should be able to sustain a specified pressure. The yield strength and density of the material is determined using some (unspecified) material simulation model. The accuracy of the model can be improved by the addition of more details about the material microstructure. However, this addition of information requires costly experiments and it is desired to avoid this cost as much as possible. Hence, the refinement question faced by the designer is “How much refinement of the material model (yield strength, and density) is appropriate for the design of the pressure vessel?”

Since the simplified material model does not model all the microstructure details, the material properties predicted from the model are imprecise. Although the predicted material properties have some errors, consider a scenario where accuracy bounds on the properties predicted by the simulation model are available. In other words, it is known with confidence that the numerical values of properties lie between a specified lower and upper bounds. It is important to note here that the imprecision in the information is not due to randomness but is a result of lack of knowledge about the system. As the accuracy of the material simulation model increases through model refinement, the bounds on predicted values decrease and the predicted numerical value of the properties change.

The first step in the stepwise refinement method proposed in Section 3.2 involves formulation of a design decision. We use the Utility-based compromise DSP construct (Mistree et al. 1993, Seepersad 2001) to formulate the design decision. The decision is shown in Table 2. Using the material information model, a designer intends to determine the following dimensions of the pressure vessel: the radius (R), length (L) and thickness (T) as shown in Figure 7. In this illustrative problem, the dimensions of length and thickness are fixed in order to make it a one dimensional problem that can be easily visualized using 2-dimensional plots.

Hence, the only design variable is the radius of the pressure vessel. Due to the manufacturing constraints, there are limitations on the maximum and minimum values of the radius. An additional constraint on the design problem is that the pressure vessel should not fail under given pressure. It is assumed that the pressure vessel is thin walled. The decision problem is a utility maximization problem with inputs of preferences, constraints, goals and associated targets, and the design variable. The material properties are shown with bold arrows depicting the imprecision due to simplified material models. Due to this imprecision, the overall utility is imprecise, and hence represented by a bold arrow.

A designer’s preferences for the attributes of weight and volume are modelled using utility functions. An overall multi-attribute utility function is formulated by taking a weighted sum of the individual utility functions for weight and volume. The multi-attribute utility function at a point in the design space (i.e., for a combination of values of design variables) is also referred to as the overall utility at that point. Due to the imprecise nature of material properties in the decision, the overall utility is also imprecise, and is associated with lower and upper bounds. The objective is to select a point in the design space that maximizes the Hurwicz criterion with a pessimism index of α=0.5.

In addition to designing the pressure vessel, the designer’s objective is also to determine the level of imprecision in the material model that is appropriate for making decisions about the pressure vessel. Beyond that level of imprecision, the cost of reducing imprecision overtakes its potential benefits in terms of making better decisions. Note that the imprecision in the material model translates to the imprecision bounds on the material properties predicted by the model. Following the method presented in Section 3.2, designers start
with a simple material model with imprecision, and sequentially refine it if the improvement potential is high. Due to the refinement of the material model, the range of material property values reduces. Further refinement of the material model stops when the improvement potential is low.

4.2 Model Refinement in Pressure Vessel Design Problem

4.2.1 Refinement of Strength Information

We first consider a design scenario where the information about the strength of the material used to manufacture the pressure vessel is imprecise. We assume that the imprecision range for strength is known, and that with addition of more information, the range of strength can be reduced. For example, in the simplest material model, the range of predicted strength values is between [50000, 650000] kPa where the first number represents the lower bound and the second number represents the upper bound. Through the addition of more information in the material model, the range reduces to [100000, 600000] kPa. In Table 3, a progression of nine such hypothetical model refinements is listed.

The imprecise strength information for each scenario in Table 3 is used in decision making to select a radius that maximizes the objective function value based on the Hurwicz criterion. The maximization of utility based on the Hurwicz criterion for Scenario 1 is shown in Figure 8. The figure corresponds to the decision making using bounds on expected utility shown in Figure 5. The lower bounds on the utility for various values of the design variable (R) are plotted as \( U_{\text{min}} \), whereas the upper bounds are plotted as \( U_{\text{max}} \). The Hurwicz utility is plotted as H, which is maximum at R=6.1 inches. The maximum value of H is denoted as \( H^* \), which is equal to 0.505 in this scenario. The corresponding point on the design variable axis is the decision point. For this particular scenario, the lower bound on the expected utility at the decision point happens to be equal to the maximum value of Hurwicz utility \( U_{\text{min}}^* = 0.505 \). The maximum utility that can possibly be achieved at any point in the design space is labelled in Figure 8 as \( \max(U_{\text{max}}) \), and is equal to 0.75. Hence, the improvement potential for scenario 1 is evaluated as:

\[
P_I = \max(U_{\text{max}}) - U_{\text{min}}^* = (0.75 - 0.505) = 0.245
\]

A designer follows the steps presented in Figure 6 to perform stepwise refinement of the simulation model, while calculating the improvement potential (i.e., the value-of-information based metric for refinement presented in this paper) at each step. The refinement is carried out until the improvement potential is sufficiently low. Although sufficiently low is a qualitative term, a designer can relate it back to the achievement of design objectives. For example, to understand the impact of \( P_I = 0.245 \) on the design objectives, we present Figure 9, which is a contour plot of overall utility as a function of the design objectives (i.e., weight and volume). Using such a contour plot, a designer can visualize the impact of a given improvement potential on the design objectives. The point that corresponds to the solution obtained from Scenario 1 is shown on the plot. An improvement potential of 0.245 implies that the overall design solution can improve within the region bounded by the dashed line. This possible improvement in design objectives can be used by the designers to decide whether it is worth refining the model (which also corresponds to whether the improvement potential is sufficiently low).

In this problem, it is observed that after a certain stage (scenario 5), although the strength is imprecise, the improvement potential goes to zero. Hence, a designer may stop reducing the imprecision interval because after this stage, any further reduction in the range for strength does no longer improve the designer’s decision-making ability. Note that the refinement potential is zero because material strength appears as a constraint in the design decision. In this problem, the maximum stress equals 156378 kPa. When the lower bound of strength exceeds this maximum stress, the constraint becomes inactive and no longer affects the decision. This is true in Scenarios 5 through 9 where the lower bound on strength is greater than the maximum stress. The
refinements after scenario 5 result in an improvement potential of zero. Hence, the answer to the refinement question posed in Section 4.1 is that the imprecise yield strength information \([16000, 54000]\) kPa is appropriate for designing the pressure vessel.

In order to illustrate the effects of further refinement on the design decision, the results of decisions made at individual refinement steps are shown in Table 3. The refinement of model is carried out until the output of the model is a precise value of \(350000\) kPa. For each refinement scenario, the expected utility at the decision point and the improvement potential are shown in Table 3. It is evident that after scenario 5, there is no effect on the design decision. The decision made in scenarios 6 through 9 is the same (Radius = 20.1 in). The design objectives (weight and volume) associated with the decision made in Scenario 5 are plotted in Figure 9. Since a designer does not need to gather additional information about material strength, the resources that would have been spent on gathering additional information are saved. Hence, the metric supports designers in making decisions in an efficient manner. This shows the advantage of the value-of-information based metric in making refinement decisions. Although this is a very simple illustrative problem, it represents similar situations that occur in more complex design problems and other optimization scenarios.

### 4.2.2 Refinement of Density Information

Since the strength information only factors as a constraint in the decision formulation shown in Table 2, the improvement potential drops to zero, providing a clear indication that further refinement of the model is not required. In this section, we assume that the density of the material used to manufacture the pressure vessel is imprecise, but strength of the material is known with certainty. The range of possible density values is known. The information about the density directly affects the objective function and hence the cDSP results. With addition of more resources, the range of possible values can be reduced. For example, in the simplest material model, the range of predicted density values is between \([0.033, 0.533]\) lb/in\(^3\). On refinement of the material model, the imprecision range reduces to \([0.080, 0.480]\) lb/in\(^3\). It is expected that the improvement potential reduces from scenarios with refinement of the material model. The reduction in improvement potential with five such refinements of the density information is shown in Figure 10. In the figure, it is observed that the improvement potential reduces at almost a constant rate until the imprecision range of density reduces to \([0.283, 0.283]\), which represents a precise numerical value. Hence, the conclusion is that for the pressure vessel design problem under consideration, although the refinement of strength information is not beneficial after a certain point, the refinement of density information is beneficial for improving the design solution. The extent of the benefit is indicated by the magnitude of the improvement potential, which depends on the complete decision formulation, including the preferences (given by utility functions for individual goals), constraints, ranges of design variables, etc. We study the impact of a designer’s preferences on the magnitude of improvement potential in Section 4.2.3.

### 4.2.3 Impact of Designer’s Preferences on Model Refinement

Consider different preference scenarios characterized by different utility functions for the weight goal (see Table 2). The accuracy of the material model is fixed. We assume that strength information is precise and the imprecision range on the density is fixed at \([0.133, 0.433]\) lb/in\(^3\). Four examples of the utility functions for the weight goal are shown in Figure 11. Each of the utility functions has a quadratic shape and is associated with an unacceptable weight beyond which the utility is zero. In order to study the effect of preferences on the Improvement Potential, 14 different decisions are formulated, each with a different unacceptable value for the weight goal. These decisions are executed independently. The results from execution of the decisions (i.e., the Hurwicz utility and the Improvement Potential) are plotted against the corresponding unacceptable weight in Figure 12.

In the figure, it is observed that the Hurwicz utility increases monotonically as the unacceptable weight increases. This is intuitive because by increasing the unacceptable weight, we are essentially relaxing the
target for weight, thereby increasing the achievement of the target. The improvement potential does not change monotonically, however. It is low when the unacceptable weight is either below 1500 lbs or above 10000 lbs, indicating a low benefit of refinement of the density model under these conditions. When the unacceptable weight is below 1500 lbs, the weight goal is highly stringent. Even with the refinement of the model the possibility of improving the overall utility is low. Hence, the improvement potential is low. When the acceptable weight is greater than 10000 lbs, the weight goal is easily achieved and with refinement of the model the possibility of improvement in the solution is low. In the scenarios where the unacceptable weight is between 1500 lbs and 10000 lbs, the improvement potential is relatively high because the possibility of improvement of solution is higher with improvement in the density information. Hence, we conclude that the decision to refine the simulation model depends significantly on the overall problem formulation, and the improvement potential helps designers in reducing the model development effort by indicating when refinement is necessary and when an approximate model is appropriate.

5. Example – Design of Materials

In this section, we present an example of simulation model refinement from the material design domain. In this design example, the objective is to design a Reactive Powder Metal Mixture (RPMM) to achieve desired properties. A mixture of aluminium and iron oxide particles in an epoxy matrix is an example of a RPMM. A designer of such materials can control material parameters such as constituent volume fractions and particle sizes to obtain desired properties. The performance of the material is defined in terms of its strength, energy release capability, etc. and is predicted by a Finite Element based simulation model. The model is imprecise and can be refined through various modes of refinement. As the model is refined, the complexity of the model and the associated runtime increases. In order to make decisions efficiently, an appropriate level of refinement of the model is desired. In this section, we show how the proposed approach can be used to determine the appropriate level of refinement of the model. Different modes of refinement of a Finite Element model are explicitly considered in this section. This is in contrast to the pressure vessel example, where the refinement was carried out hypothetically by simply reducing the parameter ranges. In order to understand the details of the materials design problem, the simulation model used to predict the material behaviour is described in Section 5.1. The design problem is discussed in Section 5.2 and the results from refinement are discussed in Section 5.3. For complete details of the problem, refer to (Panchal 2005).

5.1 Shock Simulation Model

5.1.1 Model Description

The design problem in this section is to choose appropriate values for the controllable parameters of the RPMM, in order to achieve target values of mixture properties as a shock wave propagates through the material. The model discussed in this section is used to support such a design problem by simulating the propagation of a shock wave through a RPMM. The inputs to the model include the shock speed, the dimensions of material under consideration, the volume fractions of constituents, and the size of constituent particles. Using the information about the material properties of the constituents (aluminum, iron-oxide and epoxy) as input, the model generates the overall material properties of the mixture as the shock propagates. The simulation model is developed by Austin (Austin 2005). Only the relevant details of the model are discussed here. The shock simulation consists of two steps – a) the generation of a synthetic microstructure based on experimental information, and b) the simulation of shock propagation using a Finite Element method. In the first step, information obtained from microscopy of fabricated RPMMs is used to generate information about the distribution of particles in the mixture. This information is quantified in terms of the
probability distributions for sizes and nearest-neighbourhood distances of the particles and voids. It is then used to randomly generate Statistical Volume Elements (SVEs) of micron-scale particles (i.e., aluminum particles, iron oxide agglomerates, and voids). The SVEs represent a small section of the material through which a shock is propagated. The sizes and spatial locations of the particles in the SVE are modelled such that they closely approximate the experimentally generated probability distributions.

After the particle morphology is generated, the next step is to perform a numerical simulation using finite element techniques. In this model, the properties of individual particles are used as inputs for the model. Based on the individual constituent properties, the effective properties of the mixture are determined. Specifically, the propagation of a shock wave through the reactive particle system is simulated to understand the effect of material properties and morphology on the hydrostatic behaviour of the overall mixture. The simulation is performed using an Eulerian hydrocode (RAVEN) (Benson 1995). The boundary conditions on the SVE are shown in Figure 13. The shock propagation phenomenon is idealized as a 1-D shock wave. A compressive shock wave is propagated through the mixture by applying a Lagrangian velocity boundary condition to the left surface of the SVE. The boundary on the left hand side is provided an initial velocity, called particle velocity ($V_p$). Symmetry planes serve as Lagrangian boundary conditions for the top and bottom surface of the model. A fixed Lagrangian boundary condition is imposed on the right hand side surface. Based on the results of the simulation model, the speed of the shock wave ($V_s$) is determined. The relationship between the $V_p$ and $V_s$ is used to model the hydrostatic behaviour of the mixture by employing the Gruneis Equation of State (for details of the calculation, please refer (Austin 2005)). Since the hydrostatic behaviour of the mixture is directly dependent on the shock wave speed, a designer can specify the target performance of the material in terms of the shock wave speed when the particle speed is fixed.

5.1.2 Imprecision in Shock Simulation Model

Although there are various sources of imprecision in the shock simulation model, we focus only on the imprecision that is due to the fact that a) only a small portion of the domain is modelled, and b) the domain is discretized using a finite element mesh. The material morphology in the SVE is randomly generated based on the statistical properties of the distribution of both size of particles, and the distance between them. Since the particles are randomly distributed, the material morphology is different every time a new set of particles is generated, even for the same set of parameters. The chosen size of the SVE is one of the main factors determining the imprecision in response. Smaller SVEs have more imprecision as compared to the larger SVEs. As the size of the SVE increases, the imprecision reduces because of the ‘averaging effect’. Hence, the model can be refined by increasing the size of SVE.

After the material morphology is generated, the simulation is deterministic, i.e., the same morphology with the same boundary conditions will result in the same values for the output parameters. However, since the particle shock simulation is an FEM based simulation model, there is imprecision in the outputs due to discretization also. The parameter that can be used to control imprecision due to discretization is the size of the individual cells in the 2-D mesh. Hence, the simulation model can be sequentially refined by a) increasing the size of statistical volume element (SVE) and b) reducing the size of individual cells in the finite element mesh. Hence, the refinement question faced by the material designer is “What are the appropriate values of the two model refinement parameters for designing the material?”

5.2 Description of the Materials Design Problem

From a decision making perspective, the design problem can be viewed as two decisions: a decision about the material and a decision about model refinement. In the first decision, a designer needs to choose appropriate values of the material parameters such as volume fractions of individual constituents, particle sizes, etc., whereas in the second decision, a designer is interested in choosing appropriate values of the two model
parameters (SVE size and cell size). Both these decisions depend on each other. Depending on the target requirements for material properties, the appropriateness of the level of refinement of the model may change. Similarly, depending on the level of model refinement chosen, the decision about material properties may change.

5.2.1 Material Decision

The material design decision is presented in Table 4. In this problem, we assume that the following two material parameters are variable: the size (radius) of aluminum particles and the volume fraction of voids. The objective is to achieve a shock wave speed of 4.5km/sec at which the reaction initiates. Any shockwave speed below 3.5km/sec is unacceptable and a shock wave speed greater than 4.5 has the same preference (Utility = 1). A quadratic utility function is used between 3.5km/sec and 4.5km/sec. The range of radius of aluminum particles considered is [0.5, 1.5]μm and the range of volume fraction of voids is [0.02, 0.10]. All other material parameters are assumed constant. The particle speed is fixed to 1 km/sec. The objective is to achieve the target shock wave velocity. Shock speed is chosen as an objective because the hydrostatic behaviour of the mixture is influenced directly by the shock speed. As discussed previously in this section, the material properties can be modelled using the Gruneisen Equation of State (EOS) which is determined by fitting a straight line to the particle speed versus shock speed data. Hence, the material properties are dependent on the shock speed achieved for a given particle speed.

5.2.2 Refinement decision

As mentioned before, the refinement decision involves choosing the size of SVE and the cell size. The size of SVE (S_w) is defined in terms of its length, which lies in the interval [0.014, 0.028]mm. The width is taken as half of the length in order to maintain the same aspect ratio for all scenarios. The cell size (S_c) is similarly defined in terms of its length. The length of a cell in the mesh lies within the range [0.035, 0.140] μm. The width of the cell is half of its length. The size of SVE (also referred to as window size) and the cell size can be varied continuously between the lower and upper bounds, which provides an infinite set of options of simulation model refinements. However, exploring all those options is not effective from a decision making perspective. In order to reduce the computational load, we just explore nine different simulation model refinement options. These options are generated by taking all combinations of three levels each of the size of the SVE (with lengths of 0.014, 0.021, and 0.028mm) and the cell size (with lengths of 0.035, 0.0875, and 0.14μm).

The nine options are labelled from A through I and are shown in Figure 14. The approach is to select the simplest model (window size = 0.014mm, and cell size = 0.14μm) and sequentially refine it to a level that is just appropriate for making decisions about the material properties. The refinement of the model is shown as a graph in Figure 14. In this figure, all possible paths of refinement are shown for illustrative purposes. Only one path will be followed by a designer. The dashed lines represent refinements through increases in window size and the solid lines represent refinements through reductions in cell size. The model that is most accurate is labelled as I. A designer starts with the simplest model A, and refines it sequentially using the method presented in Section 3.2. The decisions are made using the Hurwicz criterion with a pessimism index of 0.5. At each stage, the improvement potential is evaluated, and a decision is made as to whether there is a need to refine further or not.

5.3 Results from Materials Design Problem

The decisions made using the different levels of refinement of the simulation model are presented in Table 5. The results in Table 5 contain columns for the cell size in the mesh and the window size that determine the
level of refinement of the shock simulation model. The fourth column is for the maximum overall utility achieved at the decision point. The following two columns are for design variables – mean size of aluminium and volume fraction of voids. Finally, the last column indicates the improvement potential, which is the difference between the maximum overall utility that can be achieved at any point in the design space and the minimum utility achieved at the decision point. This improvement potential is used as a metric for value of information that can be achieved by refining the simulation model further. If the improvement potential is low enough, the model does not need to be refined, whereas if the improvement potential is high, there is an opportunity for improving the decision via refinement of the simulation model.

The improvement potential for different model refinement scenarios is also presented in the graph form in Figure 14. It is observed from the graph that as the simulation model is refined, the numerical value of the metric reduces because it means that the possible improvement in the solution by refining the model also reduces. This is observed in Figure 14 while going from A→B (increasing the window size) or from A→D (reduction in cell size). The improvement potential reduces from 0.338 to 0.333 by refining the model from A→B and the value reduces from 0.338 to 0.319 by refining the model from A→D. Similarly, the improvement potential reduces as the model is further refined either by increasing the window size or reducing the cell size. Note that the improvement potential is dependent only on the current level of refinement of simulation model. It does not depend on the path followed for refinement. For example, whether the refinement is carried out as A→B→E or A→D→E, the improvement potential of E is the same.

Ideally, a designer would like to select the model with the minimum possible improvement potential. Hence, the model I may appear as the best option. However, it is important to note that as the cell size is reduced or the window size is increased the computational cost also increases. As a designer refines the simulation model from A through I in Figure 14, the cost of computation also increases. Hence, there is a trade-off between the improvement potential and the associated costs. At each stage of refinement in Figure 14, a designer must compare the improvement potential against the increase in computational cost. If the added benefit apparent from the improvement potential exceeds the cost, then further refinement is appropriate. For example, the model F has an improvement potential of 0.085 (which is very low). If this improvement potential is smaller compared to the increase in cost by using model I, further refinement of the model F is not essential. Hence, in that situation, the answer to the refinement question posed in Section 5.1.2 is that a cell size of 0.0875 μm and a window size of 0.028mm results in a simulation model that is appropriate for designing the material.

As a summary, by using the value of information based approach presented in this paper, designers can sequentially refine the simulation models and calculate the potential for improvement in the decision. If the improvement potential is low, then model refinement can stop. It is important to note that the level of refinement depends not only on the accuracy of simulation models, but also depends significantly on the decisions to be made, problem constraints, and a designer’s preferences. In the illustrative pressure vessel design problem, we show that a) a reduction in the predicted range of density values improves the design decisions, and b) in spite of a certain level of imprecision in strength, designers are able to make good decisions. Hence, by using the approach presented in this paper, designers can exploit such situations and make good design decisions efficiently (with less resource utilization). In the materials design problem, the metric helps designers in gaining insights into the model refinement process. Using the metric, the designers are able to identify that the two approaches of model refinement (i.e., increasing the window size and reducing the cell size) are not independent. The designers are also able to determine the appropriate level of refinement of the Finite Element model. In other words, the metric helps designers in making informed simulation model decisions and utilize resources in an appropriate manner. Hence, the metric serves as a guide for designers in determining when to stop refining the simulation models.
6. Closure

The question posed in this paper is “How much refinement of a simulation model is adequate for design?” The qualitative answer to this question is “Simulation models should be refined to the extent that they help designers in making good decisions efficiently”. The ‘goodness’ of decisions is dependent on the satisfaction of design requirements. Although the qualitative answer to this question is useful, a quantitative answer is required to make decisions.

To provide a quantitative answer to the question, we present a Value-of-Information based metric for determining the appropriate level of refinement of simulation models. Value of information is the improvement in the overall utility value when an exact model is used as compared to a simplified model. However, due to the unavailability of exact models in most design scenarios, designers cannot directly evaluate the improvement in the overall utility. Instead of the improvement, we use an upper bound on the value of information as a metric for refinement of simulation models. The metric is called the improvement potential, and is used to determine the level of refinement beyond which the payoff from refinement is insignificant. This metric is evaluated as the difference between the maximum expected payoff (utility) that can be achieved at any point in the design space, and the lowest expected payoff (utility) achieved at the current decision point. The value-of-information metric presented in this paper is based on the assumption that information about error bounds (i.e., the lower and upper bounds on the imprecise variables) is available.

The improvement potential has the various properties that are important for making model-refinement related decisions. These properties differentiate the metric presented in this paper from existing value of information based metrics. These properties are highlighted as follows.

- The metric is a quantification of the impact of imprecision in simulation models on the design decisions via the lower and upper bounds of payoff. This allows designers to account for imprecision in addition to the statistical variability. Existing metrics do not include the effect of imprecision.
- The metric is based on the difference between maximum and minimum payoffs achieved. Hence, it also quantifies the possible variation in payoff due to imprecision. If a designer refines the simulation model in stages, the deviation in payoff reduces, which is reflected in the reduced improvement potential. This allows designers to measure the improved confidence in decisions as the imprecision range reduces.
- The metric allows designers to quantify the opportunity for improving the design solution because the metric is based on the upper bound of payoff throughout the design space. This allows designers to assess the maximum possible improvement in the design solution by addition of information via model refinement.

Hence, we believe that the metric presented in this paper is an effective tool for designers in the process of refining simulation models and utilizing them for decision making.

Acknowledgements

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Figure 1 – Decision making under a) statistical variability and b) imprecision
**Given**

An alternative to be improved through modification.

Assumptions used to model the domain of interest.

The system parameters.

- \( n \)  number of system variables
- \( p+q \)  number of system constraints
- \( p \)  equality constraints
- \( q \)  inequality constraints
- \( m \)  number of system goals
- \( g_i(X) \)  system constraint functions
- \( A_i(X) \)  system goals
- \( u_i(A_i(X)) \)  utility function for each goal
- \( U(X) \)  Overall, multi-attribute utility function

\[
U(X) = f[u_1(A_1(X)), u_2(A_2(X)), ..., u_m(A_m(X))]
\]

**Find**

System variables

\( X = X_1, ..., X_j \quad j = 1, ..., n \)

Deviation variables

\( d_i^-, d_i^+ \quad i = 1, ..., m \)

**Satisfy**

System constraints (linear, nonlinear)

\[
g_r(X) = 0 \quad r = 1, ..., p
\]

\[
g_r(X) > 0 \quad r = p+1, ..., p+q
\]

System goals (linear, nonlinear)

\[
E[u_i(A_i(X))] + d_i^- - d_i^+ = 1 \quad i = 1, ..., m
\]

Bounds

\[
X_j^{min} < X_j < X_j^{max} \quad j = 1, ..., n
\]

\( d_i^-, d_i^+ > 0 \) and \( d_i^- + d_i^+ = 0 \)

**Minimize**

Deviation function: Additive Multi-attribute Utility Function

\[
Z = 1 - E[U(X)] = \sum k_i (d_i^- + d_i^+)
\]

---

Figure 2 - Mathematical Formulation of Utility-Based Compromise Decision Support Problem (Seepersad 2001)
Value = (Ideal Maximum Payoff) – (Achieved payoff using predicted behavior)

Value = 0 (Good enough for decision making)
Value = 1 (Not appropriate for decision making)

Design Variable

Figure 3 - Conceptual description of value-of-information in simplified models
Figure 4 – Two extreme scenarios of Value of Perfect Information
Design Variable

Expected Overall Payoff (Utility)

Decision based on maximization of Hurwicz Criterion

* Refers to the decision point

\( H \) = Utility using Hurwicz Criterion

\( H^* \) = Utility using Hurwicz Criterion at Decision Point

\((U_{\text{max}})^*\) = Upper Bound expected Utility at Decision Point

\((U_{\text{min}})^*\) = Lower Bound expected Utility at Decision Point

\( \max(U_{\text{max}}) \) = Maximum of Upper Bound on Utility throughout the Design Space

Figure 5 - Decision made using bounds on payoff
1. Formulate decision using compromise DSP
2. Develop Simple Simulation Model
3. Determine Imprecision Bounds
4. Determine Decision Point, Find Lower Bound of Expected Utility
5. Determine Upper Bound of Expected Utility in Design Space
6. Evaluate Improvement Potential
   \[ P_I = \max(U_{\text{max}}) - \min(U_{\text{min}}) \]
7. Refine Simulation Model

Figure 6 – Method for Stepwise Refinement of Simulation Model
Figure 7 – Thin walled pressure vessel (Lewis and Mistree 1997)
Strength = [50000 650000], R = 6.1, H* = 0.50467, P_I = 0.24454

Figure 8 - Illustration of decision making in Scenario 1 of pressure vessel design problem
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<thead>
<tr>
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<th>Radhakrishnan and McAdams (Radhakrishnan and McAdams 2005)</th>
<th>Bradley and Agogino (Bradley and Agogino 1994)</th>
<th>Poh and Horvitz (Poh and Horvitz 1993)</th>
<th>Augenbaugh and co-authors (Augenbaugh et al. 2005)</th>
<th>Panchal and co-authors (this paper)</th>
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<tr>
<td>Model selection in Engineering design using a utility based approach</td>
<td>Selection of alternatives under uncertainty during conceptual design</td>
<td>Refinement of decision problem formulation</td>
<td>Refinement of probability distributions on experimental data</td>
<td>Refinement of simulation models by quantifying the impact of reduction in imprecision on design decisions</td>
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</table>
Table 2 - Decision formulation for Pressure Vessel problem using cDSP (imprecise strength, precise density)

**Given**
- Strength ($S_t$) = [50000, 650000] kPa
- Pressure ($P$) = 3890 kPa
- Density ($\rho$) = 0.283 lb/in$^3$
- Length ($L$) = 90 in
- Thickness ($T$) = 0.5 in

**Relation for Volume and Weight:**
- Volume, $V = \pi \left[ \frac{4}{3} R^3 + R^2 L \right]$
- Weight, $W = \pi \rho \left[ \frac{4}{3} (R + T)^3 + (R + T)^2 (\frac{4}{3} R^3 + R^2 L) \right]$

**Find**
- System variable: Radius ($R$)

**Satisfy**
- System constraints:
  - $S_t - \left( \frac{PR}{T} \right) \geq 0$
  - $R - 5T \geq 0$
  - $(40 - R - T) \geq 0$
  - $(150 - L - 2R - 2T) \geq 0$

**Utility Functions for Volume and Weight**
- $U_W = 1 - 0.6 \left( \frac{W}{4000} \right) - 0.4 \left( \frac{W}{4000} \right)^2$
- $U_V = 1.4 \left( \frac{V}{150000} \right) - 0.4 \left( \frac{V}{150000} \right)^2$
- $U_{Overall} = 0.5U_W + 0.5U_V$

**Bounds on Radius:**
- $R = [1, 36]$

**Minimize**
- Deviation from Maximum Utility:
  - $Z = (1 - U_{Overall})$
### Table 3 - Results from refining strength model

<table>
<thead>
<tr>
<th>Scenario No.</th>
<th>Lower Bound (kPa)</th>
<th>Upper Bound (kPa)</th>
<th>Radius (in)</th>
<th>Utility using Hurwicz criterion</th>
<th>Improvement Potential</th>
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<td>650000</td>
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<td>350000</td>
<td>20.1</td>
<td>0.749</td>
<td>0.000</td>
</tr>
</tbody>
</table>
Table 4 - Material design decision

Given
Cell Size ($S_c$) = [0.035, 0.140] microns
Window Size ($S_w$) = [0.014, 0.028] mm
Particle Speed ($V_p$) = 1 km/sec

Particle Shock Simulation Model

$v_b = f(R, VF, S_c, S_w)$

(that predicts shock speed as a function of Radius of Aluminum, Volume Fraction of Voids, Cell Size, and Window Size)

Find

Values of design variables
Size of Aluminum Particles ($R_{Al}$)
Volume Fraction of Voids ($VF_{void}$)

Satisfy

Bounds on design variables
Size of Aluminum Particles = [0.5, 1.5] μm
Volume Fraction of Voids = [0.02, 0.10]

Preference for shock wave speed

$u_{overall} = u_c = \begin{cases} 
0, & V_s \leq 3.5 \\
1.4(V_s - 3.5) - 0.4(V_s - 3.5)^2, & 3.5 < V_s < 4.5 \\
1, & V_s \geq 4.5 
\end{cases}$

Minimize

Deviation from Maximum Utility:

$Z = (1 - U_{overall})$
Table 5 - Decision outcomes for different refinement scenarios

<table>
<thead>
<tr>
<th>Refinement Case</th>
<th>Design Variables</th>
<th>Value Metric</th>
</tr>
</thead>
<tbody>
<tr>
<td>Label</td>
<td>Cell Size (microns)</td>
<td>Window Size (mm)</td>
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<tr>
<td>A</td>
<td>0.1400</td>
<td>0.014</td>
</tr>
<tr>
<td>B</td>
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</tr>
<tr>
<td>C</td>
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<td>D</td>
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