

## THE RELIABILITY OF COMPUTER PREDICTIONS: CAN THEY BE TRUSTED?

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**Abstract.** The issue of reliability of computer predictions of physical events is examined as the goal of verification and validation processes. It is argued that verification, both solution and code verification, can be carried out with a high degree of confidence, even though much remains to be done to improve and advance verification procedures. It is validation of mathematical models that stands as the major bottleneck of reliable computer predictions. Uncertainty of input data represents a major feature of validation processes and must be quantified if models are to be judged valid or invalid. Examples are given from solid mechanics and heat transfer that demonstrate validation processes employing stochastic models and fuzzy set theories.

**Key Words.** Verification, validation, computer simulations.

### 1. Introduction

Computational Science (CS) is the discipline concerned with the use of computers and computational methods to simulate physical events and to make quantitative predictions of physical phenomena. Such predictions are often used as a basis for critical decisions effecting the health, security, and well being of humankind. For this reason, CS has had a major impact on many fields in engineering, physics, chemistry, health sciences, economics, finance, politics, and other areas. The great promise that CS will be of immense value to all areas of science and technology depends on a crucial factor: the reliability of computer products and our ability to measure in some way this reliability [34].

In a recent report, Post [38] speaks of the coming crisis in CS arising from three major challenges: a) performance, b) programming, and c) prediction. We agree with Post that the performance and programming challenges have been met or will be met soon, but the prediction challenge will require considerable advancement and maturity in the way that simulation is done and interpreted.

Concerning performance, a look at the history of computer performance over the last one-and-a-half decades gives weight to the viewpoint that the so-called "performance challenge" of CS is well in hand. Using the 11/780 VAX as a unit measuring computer capabilities a decade before the end of the twentieth century (1989), the unit involves one megabyte of memory, a half gigabyte of disk storage, and one cpu with a speed of 0.1 megaflops. In 1992, three years later, the IBM

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RS580 had 54 times the memory of the VAX and its speed was 1000 times greater. In 1997, eight years later, the SGI Power Challenge had 1000 times the memory of a VAX, six cpu units with a theoretical speed of 18,000 times that of the 1989 VAX. In November of 2004, IBM's Blue Gene/L supercomputer became operational with an expected peak performance of  $36.0 \times 10^{12}$  flops, over a hundred million times faster in unit capability than the VAX. Today, \$1000 can buy a computer as powerful as the biggest and most capable computer available at any cost in 1990. Experts predict that Moore's law will continue to hold for 15-20 years so that this exponential growth in performance will continue [21]. These data convince us that the performance challenge is being met.

The programming challenge, supplying the software to keep up with hardware developments, is also being met, albeit at a slower pace. Significant progress in the development of new languages and new devices gives confidence that the programming challenge is being reasonably addressed and can be met even more vigorously in the years ahead.

The prediction challenge, which is at the heart of CS, is viewed as the most difficult challenge to be met in the future, and stands as a major bottleneck, perhaps a crisis, in CS. Again, the major issue is the reliability of computer predictions and their use as a basis for important decisions.

In the present paper, we will discuss the prediction challenge, comment on various mathematical aspects of it, and point to some serious limitations of contemporary methods of computer prediction. We will also address the question of what machinery must be developed in order to use such predictions to make meaningful decisions.

## 2. Verification and Validation in CS

Verification and Validation (V & V) has emerged in recent years as the intellectual and technological discipline that addresses the prediction challenge. Both are processes, verification being the processes addressing the quality of the numerical approximation of the mathematical model used as the basis for a prediction, and validation being the process addressing the reliability of the mathematical model as a faithful abstraction of reality. V & V has been the focus of much study and debate in recent years and a relatively large literature exists and is expanding (e.g., [19], [23], [33], [39], [42]).

In [11], we present a detailed list of definitions and concepts related to V & V. Worthy of mentioning here are the following:

- *physical event*: an occurrence in nature, a fundamental entity of physical reality
- *simulate*: to build a likeness; in our case, the likeness is produced by the interpretation of prediction results produced by a computer
- *mathematical model*: a collection of mathematical constructions that provide abstractions of physical events, based on scientific theories covering the event, and available input information
- *computational model*: a discrete approximation of a mathematical model rendered in a form manageable by a computer or an appropriate computing device.

A typical example of a mathematical model is the set of equations and conditions characterized by a boundary value problem involving deterministic or stochastic differential equations together with functionals defining quantities of interest. These quantities of interest are the goals of the computer prediction, which, in turn, are the basis for decisions.

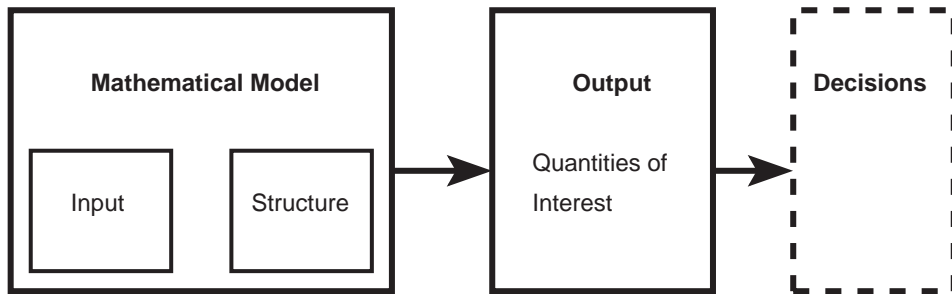


FIGURE 1. The scheme of the mathematical problem

The mathematical problem is described by its structure and its input data. The structure of the mathematical problem comprises functional relations between the input and the output. For example, the structure can be expressed by a system of conservation laws. The input data is the set of all admissible data needed for solving the mathematical problem. For example, input data includes the classic boundary conditions and parameters used in the structure of the problem. The data also include the characterization of the uncertainty as when it is part of the mathematical problem. We will include as part of the mathematical problem the quantitative characterization of the uncertainty in the predicted quantity of interest.

In the literature the term mathematical problem and mathematical model are not distinguished, although the term model is often used in a more generic sense than mathematical problem, which involves all input data. We will not distinguish between the *problem* and the *model* either. Symbolically, the mathematical problem can be viewed as shown in Figure 1.

It is worthwhile to distinguish between the general mathematical problem and a specific one which employs specific input data. This specific problem then leads to the desired prediction. In this case, we speak of the prediction problem. Validation problems, introduced later, are also specific problems for some input data, which are different from the prediction problem. The validation problem, of course, must have some features in common with the prediction problem.

A mathematical problem is a mapping of the space (set) of input into the output space. From this point of view, every mathematical problem is, in a sense, deterministic because any uncertainty is described in a deterministic way. This is accomplished, for example, by using the parameters defining the probability density, by using Karhunen-Loeve expansions or characterizing ignorance by specifying the membership functions of fuzzy set theory.

In the literature, simulation is sometimes presented without a reference to any mathematical problem. Nevertheless, if the simulation of a physical event has to be independent of various computational parameters and procedures which are not directly related to the physical event of interest, then a mathematical problem has to be in the background, so that it is always possible to speak of accuracy, convergence, etc.

We would like to underline that in reality the input data always contain uncertainties not taken into account in classical deterministic modeling.

*Identification* is the process of obtaining input data for a specific problem, for example for the prediction problem. They are obtained by various means, for example, by fitting the data from calibration experiments.

*Uncertainty, variability and ignorance.* We have to distinguish between objective uncertainty, addressing variability (aleatoric uncertainty), and subjective (or epistemic) uncertainty. We use the term ignorance to denote the partial incertitude that arises because of the limits of knowledge. For example, variability in the coefficients of a partial differential equation can be described in a probabilistic way using known probability fields obtained from experiments. We will speak of *ignorance*, if the probability field is characterized by expert opinions. In most practical cases, different levels of ignorance are always present. Insufficient input information is often available due to, for example, the absence of experimental data, in which case one must rely on the opinions of experts. Often the reliability of a prediction is more influenced by ignorance than by variability. The quantitative characterization of uncertainty, either variability or ignorance, is a major problem. In this paper, we speak in general about uncertainty, but more precisely, we will use the terms variability and ignorance when appropriate.

*Verification* is the process of determining if a computational problem and the code implementing the computational problem leads to a prediction of sufficient accuracy, i.e., the difference between the exact and computed quantity of interest is sufficiently small. Hence, verification has two aspects, the approximation aspect and the verification of the correctness of the code, i.e., the program developed to implement the computational model can faithfully produce the intended results. Although code verification is obviously essential, we will not address it in the present paper. The first part of verification, so-called *solution verification*, is essentially a problem of *a-posteriori* error estimation. It addresses not only classical methods of error estimation of standard approximation methods (such as finite elements) but also errors due to simplification of the problem. For example, errors due to the linearization of a nonlinear problem or of dimensional reduction, or the error in the simulation produced by Monte Carlo methods because, as said above, there is always a mathematical problem in the background.

*A posteriori* error estimation is a fairly mature subject and many techniques for developing *a-posteriori* error estimates have been proposed in the literature, e.g., [1], [12], [13], [35], [36]. *A posteriori* error estimation is a purely mathematical process and, while many open problems remain, effective methods exist for addressing solution verification for a large class of computational models.

*Validation* is the process of determining if the mathematical model of a physical event (the prediction) represents the actual physical event with sufficient reliability. In contrast to the verification, validation addresses the problem how well the theory describes reality. This question is related to a major problem in philosophy, especially in the philosophy of science. A first question is what is actually meant by validation and whether validation is even possible. The related question of whether a scientific theory can be validated was addressed by the eminent twentieth century philosopher Karl Popper [37]. For more discussion of this point, see also [11]. In the validation procedure, we consider a set of validation problems. These problems are specific mathematical problems for which some of the input data are the same as those in the prediction problem, but others may be different. For example, in the elasticity problem, the domain and the boundary conditions are different for the validation and the prediction problem, but the constitutive law is the same. These validation problems are simpler than the prediction problems and can, in general, be experimentally studied.

**Remark** In addition to the relatively simple validation test, one very complex and expensive validation test, called the accreditation test is sometimes used. We note that it is still not so complex as the prediction problem.  $\square$

An issue of fundamental importance is to develop a plan for validation in the absence of experimental data or for cases in which only incomplete data are available. In such cases, a systematic approach toward quantifying ignorance has to be considered using, for example, fuzzy set theory or comparable approaches. Instead of experimental data, expert opinion has to be used as a basis for assessing the validity of models and quantifying uncertainty.

**Remark.** Experimentation also involves analogs of verification and validation. The accuracy of measurements is analogous to verification while validation relates to the question of whether the experiment measured what was intended.  $\square$

In the validation process, the computed predictions of the measured data are compared with the actual measured data or the experts expectation. If they differ too much in a given metric for the criterion used, then the (prediction) models are rejected. If a sufficiently large set of validation problems is not rejected, then the prediction problem is considered to be validated and it is assumed that the accuracy (or likelihood) of the prediction is close to the accuracy of the predictions in the validation problems. The metric used and the criterion for comparison has to be closely related to the prediction problem and its goals.

The validation process can be broad and not confined to simply testing assumptions made in the formulation of the mathematical model. For example, the validation process could be designed to also assess the reliability of the techniques for quantifying uncertainty in the context of the quantity of interest, as well as to assess the robustness of the model regarding its sensitivity to uncertainties. The selection of the validation problems and metrics is not an easy problem. It has mathematical and experimental aspects and, because of the cost of experiments, financial aspects that have to also be considered.

The prediction and validation problems are always different because the prediction problem is not accessible to experiments. If experiments on the original prediction problem are actually carried out, then their comparison with predictions is referred to as a *post-audit* and the prediction reduces to another validation problem.

Because of today's powerful computers, verification is often an achievable possibility for an increased computational cost. Validation is then the bottleneck in assessing the reliability of computer predictions.

In the following sections we address three specific problems which illustrate various basic possibilities occurring in prediction problems.

### 3. Examples of Models of Physical Events

- (1) A problem in which experimental data are insufficient and ignorance is present. We will demonstrate the use of quantitative fuzzy set characterizations of the ignorance.
- (2) A problem in which sufficient experimental data are available to lead to the rejection of the most commonly used models of plasticity.
- (3) A problem in which the variability is fully known by its probability field.

**3.1. Quasi-Static Problems in Solid Mechanics.** As a first example, we consider events modeled as the quasi-static deformation of a deformable body with material points  $\mathbf{x}$  in a bounded domain  $\Omega \subset \mathbb{R}^3$  subject to time-independent or cyclic boundary conditions. The quantities of interest are specified below. We will

assume that the boundary data are sufficiently small so that the standard assumption of small displacements is valid. The mathematical problem is to find certain quantities of interest, which may depend upon the displacement field  $\mathbf{u}$ , the stress tensor  $\boldsymbol{\sigma}$  and the strain tensor  $\boldsymbol{\varepsilon}$  which satisfy

$$(3.1) \quad \operatorname{div} \boldsymbol{\sigma}(\mathbf{x}, t) = 0 \quad \boldsymbol{\sigma} = \{\sigma_{ij}\},$$

$$(3.2) \quad \boldsymbol{\sigma}(\mathbf{x}, t) = \mathcal{A}(\boldsymbol{\varepsilon}(\mathbf{x}, \tau)), \quad 0 \leq \tau \leq t,$$

$$(3.3) \quad \begin{aligned} \boldsymbol{\varepsilon} = \{\varepsilon_{ij}\}; \quad \varepsilon_{ij} &= (\partial u_i / \partial x_j + \partial u_j / \partial x_i) / 2 \\ \mathbf{x} &\in \Omega \subset \mathbb{R}^3, \quad t \in (0, T), \end{aligned}$$

and boundary and initial conditions,

$$(3.4) \quad \begin{aligned} \mathbf{u} &= \mathbf{0} \text{ on } \Gamma_D \subset \partial\Omega, \\ \mathbf{T}(\mathbf{u}) &= \mathbf{T}_0(\mathbf{x}, t) \text{ on } \Gamma_T \subset \partial\Omega, \end{aligned}$$

where  $\mathbf{T}_0(\mathbf{x}, t)$  are the prescribed tractions.

$$(3.5) \quad \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), \quad \mathbf{x} \in \overline{\Omega}$$

Here,  $\mathcal{A}$  represents a functional characterizing the constitutive law of the material. In the case of linear elasticity, we have

$$(3.6) \quad \sigma_{ij} = C_{ijkl} \varepsilon_{kl}; \quad 1 \geq i, j, k, l \leq 3$$

where  $C_{ijkl}$  is the standard elliptic fourth-order tensor of elasticities and the usual summation convention is employed.

In the case of the plasticity, we consider a family of constitutive laws based on the use of the internal variables and two basic assumptions: the existence of a convex yield surface and the normality condition (the plastic strain increment during plastic flow is proportional to the outward normal to the yield surface).

We denote by  $\mathbf{T}_0$  the traction vector defined on a portion  $\Gamma_T$  of  $\partial\Omega$  and the quantities of interest, denoted,  $Q$  are functionals which specifically are defined later.

**3.2. The Heat Conduction Problem.** Consider the boundary-value problem,

$$(3.7) \quad \operatorname{div} a(\mathbf{x}) \operatorname{grad} u = f \quad \text{on } D \subset \mathbb{R}^3,$$

$$(3.8) \quad u = 0 \quad \text{on } \partial D.$$

When  $a(\mathbf{x})$  represents the thermal conductivity at a point  $\mathbf{x}$  in a bounded domain  $D$ ,  $u(\mathbf{x})$  is the temperature at  $\mathbf{x}$ , and  $f$  is a heat source, then (3.7) and (3.8) represent the classical model of diffusive heat conditions in  $D$ . This is a generic formulation of the mathematical problem wherein the assumptions on the input data and the solution are not specified there. A specific problem will be addressed in Section 6.

#### 4. Specific Elasticity Problem. Uncertainty, Variability and Ignorance

There are many ways to address uncertainty, depending what information is available. We will restrict ourselves to a few specific examples.

**4.1. The linear elasticity problem.** The input data are:

- (1) The domain
- (2) The elasticity tensor - the constitutive law
- (3) The tractions  $\mathbf{T}$

We will assume that the tractions are time-independent. All input data have uncertainties. The significance of the uncertainty depends on the quantities of interest.

- (1) **The domain.** The definition of the domain invariably includes uncertainties; for example, when the domain is given by the digital image with a pixel representation of the boundary [7], or if the domain is generated using a CAD system. Another example involves models of thin shells, where in the actual fabrication, the variation in the thickness is uncertain and can be a major part of the uncertainty in the prediction (see [42]). Here we will assume that the uncertainty in the domain has negligible influence on the quantity of interest.
- (2) **The constitutive law.** For the elasticity example, we assume that the material is the aluminum alloy, 5454 in the H 32 temper. It is essentially isotropic, although depending on the manufacturing process and rolling, some anisotropy is always present. We will assume that the material is isotropic and that the elasticity properties are characterized by only the modulus of elasticity  $E$  and the Poisson ratio  $\nu$ .

In the standard literature on mechanical properties of aluminum, only the values of the modulus of elasticity and Poisson ratio are given without any information about their statistics. See, for example, [2], [3], [31], [43]. We will assume that the published values of  $E$  and  $\nu$  are mean values of some statistical distribution. In Table 1, data taken from [8] are reproduced. Here the sheet has a nominal thickness of 0.2 inches and the plate has a nominal thickness of 0.4 inches.

TABLE 1. **Basic Properties of Aluminum Alloy 5454 in H32 Temper.**

	$S_y$ psi	$S_u$ psi	Elong %	RA %	E psi	$\rho$
Plate	25.5	40.0	17.6	28.1	10,000	1.6
Sheet	31.1	42.6	15.7	26.6	10,400	1.4

In Table 1,

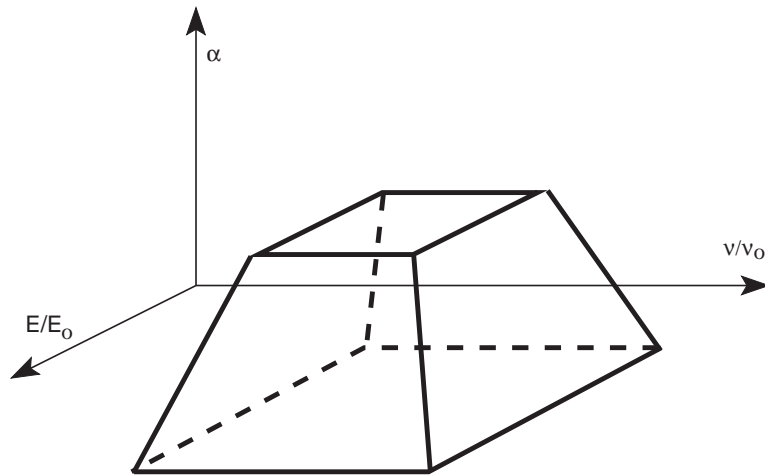
$S_y$  is the tensile yield strength

$S_u$  is the ultimate strength

$Elong$  is the elongation

$RA$  is the reduction in area

$E$  is the modulus of elasticity

FIGURE 2. The membership function for  $A^\alpha$ 

$\varrho$  is the ratio  $S_u/S_y$  which is a rough indicator of the strength hardening.

The Poisson ratio is not reported in [43]. From [31], data suggest that it is not too dependent on the thickness and has a value,  $\nu = 0.33$ .

**Remark.** The modulus of elasticity and the Poisson ratio are usually determined from classical dog-bone experiments. Measuring Poisson ratio is more difficult than the modulus of elasticity because it is defined as the ratio of two strains. Hence, the Poisson ratio could have, in general, a larger uncertainty due to the measurement error.  $\square$

Because the data variability in  $(E, \nu)$  is not known, uncertainty must be treated as ignorance. We will describe it here using fuzzy set theory, specifically through the use of so-called  $\alpha$  cuts; see, for example, [4], [20], [24], [29].

Denoting the nominal values of the modulus of elasticity and Poisson ratio by  $E^0$  and  $\nu^0$ , we will assume that in our specific problem the  $\alpha$  cuts are given by

$$(4.1) \quad A^\alpha = \left\{ (E, \nu) \left| \begin{array}{l} \frac{|E - E^0|}{E^0} \leq \beta_E, \quad \frac{|\nu - \nu^0|}{|\nu^0|} \leq \beta_\nu \text{ for } \alpha = 1; \\ \frac{|E - E^0|}{|E^0|} \leq \beta_E(2 - \alpha), \quad \frac{|\nu - \nu^0|}{|\nu^0|} \leq \beta_\nu(2 - \alpha) \text{ for } 0 \leq \alpha \leq 1 \end{array} \right. \right\}$$

where  $\beta_E = 0.01$  and  $\beta_\nu = 0.04$ . In Figure 2, we show the associated membership function. The value  $\alpha$  expresses quantitatively the likelihood that  $(E, \nu)$  is in the set  $A^\alpha$ .

We have no information about the correlation between the values of  $E$  and  $\nu$  at different points of the material. Hence we will assume these parameters have  $\alpha$  cuts independent of the positions of material points.

- (3) **The tractions.** Traction represents the effects of the outside environment on the boundaries of the body. These data are determined by independent tests, codes, other numerical calculations, or, as is often the case, they



are specified within standard regulation documents such as construction-design codes. In many cases, they are specified by the analyst. Typically, several sets of different tractions are considered in a simulation. Thus, in general, tractions can include large uncertainty and ignorance. Very often the reliability of a prediction is heavily influenced by the ignorance in the boundary conditions.

In this example, we characterize the ignorance in tractions once more by fuzzy theory. Let  $\Gamma_T = \cup_{\ell=1}^3 \Gamma_T^\ell$ . We will assume that the membership functions set of the traction  $\mathbf{T}$  is

$$(4.2) \quad A^\alpha \left\{ \left\langle \|\mathbf{T}\|_{L^2(\Gamma_T^1)} \leq 30, \text{ with } \alpha = 0.3 \right\rangle, \left\langle \|\mathbf{T}\|_{L^2(\Gamma_T^2)} \leq 10, \text{ with } \alpha = 1.0 \right\rangle, \right. \\ \left. \left\langle \|\mathbf{T}\|_{H^1(\Gamma_T^3)} \leq 50 \text{ with } \alpha = 0.7 \right\rangle \right\}$$

where  $\alpha$  is the degree of membership which quantifies the likelihood. For simplicity we will address two cases separately:

- (1) The nominal traction  $\mathbf{T}$  is completely known and the uncertainty is only in the material properties  $E, \nu$ .
- (2) The material properties with nominal values  $E^0, \nu^0$  are completely known and the uncertainty is only in the traction  $\mathbf{T}$ .

Let

$$(4.3) \quad \Omega = \{|x_1| < 4 = \ell_1, 0 < x_2 < 20 = \ell_2, |x_3| < 2 = \ell_3\} \quad (\text{inches})$$

and denote by  $Q_1$  and  $Q_2$  the quantities of interest,

$$(4.4) \quad Q_1 = \frac{1}{|S_1|} \int_{S_1} u_3 \, dx_1 dx_3, \quad S_1 = \{0 < x_1 < 4, x_2 = 20, |x_3| < 2\}$$

$$(4.5) \quad Q_2 = \frac{1}{|S_2|} \int_{S_2} u_2 \, dx_1 dx_3, \quad S_2 = \{0 < x_1 < 4, x_2 = 20, 0 < x_3 < 2\}$$

where  $u_i$  are the components of displacement.

Let  $E^0 = 10,400 \text{ psi}$ ,  $\nu^0 = 0.33$  and  $(E, \nu)$  belong to the  $\alpha$  cuts defined by (4.1) with  $\beta_\nu = 0.04$  and  $\beta_E = 0.01$ . Further let

$$(4.6) \quad \Gamma_D = \{x \mid |x_1| < 4, x_2 = 0, |x_3| < 2\}, \quad \Gamma_T = \partial\Omega - \bar{\Gamma}_D \\ \Gamma_T^* = \{x \mid |x_1| < 4, x_2 = 20, |x_3| < 2\}$$

and

$$(4.7) \quad \mathbf{T}_0 = (t_1, t_2, t_3), \quad t_1 = t_2 = 0, \quad t_3 = 1 \text{ on } \Gamma_T^* \\ \mathbf{T}_0 = 0 \text{ on } \Gamma_T - \Gamma_T^* \\ u = 0 \text{ on } \Gamma_D$$

Then the mathematical problem reads: *based on the weak solution of the boundary value problem (3.1)-(3.6) and (4.1)-(4.6), find the  $\alpha$  cuts for the quantities of interest  $Q_1$  and  $Q_2$ .* We observe that the problem is an optimization problem (in this context, the term anti-optimization could also be used) because we seek the range of values of  $Q$  when  $(E(\mathbf{x}), \nu(\mathbf{x}))$  belong to the  $\alpha$ -cut for every  $\mathbf{x} \in \Omega$ .

This problem, its theoretical properties and its numerical solution was analyzed in detail in [10]. The numerical treatment was based on first-order perturbation theory with an estimate of the influence of this approximation. The p-version of

finite element method was used and an *a-posteriori* error estimation was computed, so that the verification was also addressed.

Denoting by  $\bar{Q}_i$ ,  $i = 1, 2$ , the values of the quantity of interest functional for the nominal elasticity properties, it is shown in [10] that the  $\alpha$  cuts for  $q_i = Q_i/\bar{Q}_i$  are

$$A_i^\alpha = \begin{cases} \{q_i \mid |1 - q_i| \leq \gamma_i, \alpha = 1\} \\ \{q_i \mid |1 - q_i| \leq \gamma_i(2 - \alpha), 0 \leq \alpha \leq 1\} \end{cases}$$

where

$$\gamma_1 = 0.0153, \quad \gamma_2 = 0.0159$$

Because the perturbation approach was used, reasonable accuracy can be obtained when the ignorance is not too large, as in our prediction problem.

**Remark.** The approach used here is obviously very close to the worst case scenario approach. This is addressed in [27].  $\square$

In the second case, when the elasticity parameters are completely known and ignorance pertains only to the tractions, the problem is similar but is much simpler. For example, it is not necessary to assume that ignorance is small. We refer to [10] for more details.

## 5. Summary Observations for the Elasticity Example

We list as follows several key remarks on validation of the linear elasticity model:

- (1) Because we did not have enough information available on the modulus of elasticity and the Poisson ratio, we assumed that they could range arbitrarily and independently at every point  $\mathbf{x}$ . It can be shown that the pair  $(E(\mathbf{x}), \nu(\mathbf{x}))$  which gives the value of  $Q_i$  at the boundary of  $A^\alpha$  are piecewise constant functions [10]. Of course, other admissible sets could be used. For example, instead  $\frac{|E - E^0|}{E^0} < \beta_E$  in (4.1) we could consider  $\|E - E^0\|_{L^\infty} + c\|E - E^0\|_{W_1^\infty} \leq \beta_E E^0$ .
- (2) The uncertainty in the prediction is mainly influenced by the large uncertainty in the tractions.
- (3) We have assumed a homogeneous Dirichlet boundary condition on  $\Gamma_D$ . Obviously, this is generally an approximation because, in reality, boundary constraints against motion are almost always deformable in some sense. This could have a large effect on the quantity of interest when  $\ell_2/\ell_1 \gg 1$ . Hence, a more detailed analysis of this approximation is needed either experimentally or by computational virtual experimentation. Obviously, in this case the uncertainty will also be mainly ignorance.
- (4) We do not see here a standard validation process because essentially no experimental data are available. Nevertheless, the  $\alpha$  cuts give a very good indication of the likelihood of variations in data and of the possible need for additional experimental data or for the necessity of increasing the safety factor when making decisions.
- (5) We could also have statistical information about the coefficients and the tractions which can also be combined with the ignorance. We will discuss this in Section 6 for the heat conduction problem when the conductivity coefficient will be a stochastic function.
- (6) We used fuzzy set theory for the characterization of ignorance. There are other possibilities; for example evidence theory or possibility theory can be used (see e.g. [26]).
- (7) There are many open mathematical problems related to the mathematical and computational models addressed here. These include the treatment

of various classes of uncertainties in the elastic properties and tractions, which could be large, *a posteriori* estimates of modeling error, formulation and analysis of the boundary condition treated as a Dirichlet boundary condition, and modeling the environment from which traction boundary conditions are produced.

**5.1. The elasto-plasticity problem for cyclic loads.** We will consider here plasticity problems based on the constitutive laws satisfying the assumptions spelled out in Section 3.1. The constitutive law is the major source of uncertainty in the prediction. There are many constitutive laws proposed in the literature; see for example [17] and [44]. We will address here only the validation of the constitutive law in one dimension when experimental data and computational analysis are accessible. Even in this case, relatively little statistical data is generally available.

The theory and numerical treatment of plasticity problems without uncertainties in two- and three-dimensions is addressed in the literature (e.g., [25], [28], [30], [32]). We will now report on the basic data from [8] where many more data and details are given. The validation problems are the standard dog-bone domains which are used for experiments for determining mechanical properties of materials.

Consider an aluminum alloy 5454 in H32 temper dog-bone specimen, clamped at each end, and suppose that a strain  $\varepsilon(t)$  is imposed and the associated stress  $\sigma(t)$  (which is the quantity of interest in the validation problem) is measured and computationally predicted when a particular constitutive law is used. Strain histories are recorded corresponding to quasi-static behavior. The following strain histories are prescribed:

- a. cyclic constant-amplitude piecewise-linear strain functions with 1000 reversals, with means -0.006, -0.004, ..., 0.006 and the range 0.01.
- b. a random-amplitude piecewise-linear strain function with the same mean levels and peaks selected as random numbers with uniform probability distribution in the interval [-0.005, 0.005] and 1000 reversals.

Always two samples with the identical histories are used and all together 84 samples are investigated.

The prediction problem is two- or three-dimensional with a given quantity of interest. The selection of the validation metric defines on the prediction problem. It has to be such that the accuracy of the prediction is similar to the accuracy of the validation measured in the particular metric used.

We select a metric which is related to the  $L^\infty$ -norm. The reason is that in the linear case, which is a special case, we validate the errors in the elasticity coefficients; then the error in the solution measured in the  $H^1$ -norm is directly related to the errors in the coefficients measured in the  $L^\infty$ -norm. The metric used has to be robust in the sense that it leads to a reasonable reproducibility measure. Of course, various metrics could be used when there is an expectation (proof) that the error in the constitutive law measured in the metric will lead to the error in the quantity of interest of approximately the same size.

Denoting by  $\varepsilon$  the strain,  $\sigma_m$  the measured stress and,  $\sigma_c$  the computed stress, (the stress is the quantity of interest), we define the metric for accuracy in the constitutive law  $k$  in the window  $\Gamma^I$  as follows:

$$(5.1) \quad \Theta_k^{(i)} = \frac{\|\sigma_m(\varepsilon(t)) - \sigma_c(\varepsilon(t))\|_{L^\infty(\Gamma^i)}}{\frac{1}{2}\|\sigma_m(\varepsilon(t)) + \sigma_c(\varepsilon(t))\|_{L^\infty(\Gamma^i)}}$$

Here  $\Gamma^i$  denote the windows of different strain histories of the cycles range, (0,10), (0,20), ..., (0,200), (0,500), (10,20),..., (200,500). The denominator in (4.8) is chosen to define the metric relative to an average of  $\sigma_m$  and  $\sigma_c$  in  $L^\infty(\Gamma^i)$ .  $\sigma_m$  and  $\sigma_c$  are close together. The given model is also used as a reproducibility measure. Obviously, a relative measure has to be used. It should express that for small  $\sigma$ , respectively  $\epsilon$ , below the yield, the theory represents reality well while for large  $\sigma$  the reliability is small. This measure is in some way related to the error in the effective elasticity modulus, which is the equivalent relation between strain and stress when they exceed the yield. It is also used for iteration purposes.

The same metric is used to measure the reproducibility accuracy when two measurements with the identical strains are compared. In [8], the mean, min., max., and standard deviation of the reproducibility metric are reported. They are in the ranges 4.15-5.15, 2.4-4.3, 6.00-6.70, and 0.96-1.33. These ranges describe the variability of the material and, among other things, show that the metric is robust. In [8], four constitutive laws are analyzed:

a. *The kinematic hardening law.* This law is characterized by four numerical parameters: modulus of elasticity  $E$ , the modulus of plasticity  $E_P$ , the yield stress  $\sigma_y$  and one internal variable  $\alpha$  with its initial value. This law is very often used.

b. *The isotropic hardening law.* This law is also characterized by the three parameters and one internal variable as in case (a). Usually the kinematic law is preferred because it respects Bauschinger effects.

c. *The Chaboche law* [18]. This law has six numerical parameters and four internal variables with their initial values.

d. *The B-L law.* This law has six numerical parameters and two internal variables with their initial values.

All of the constitutive laws except the Chaboche law can be extended into higher dimensions. The B-L law is similar to the Chaboche law. The exact mathematical formulation of the four constitutive laws is given [8].

We will validate the above constitutive laws for the input data computed from the published data and zero initial conditions for internal variables. How these values were determined is explained in [8]. In the Table 2, we report the statistics of the metric  $\Theta_k^{(i)}$  for the window (0,500) for the first three of the above mentioned constitutive laws. Data for the B-L law was not available in the literature

TABLE 2. Statistics of  $\Theta_k^{(i)}$  for the parameters determined from published data.

	a		b		c	
	CONST	RAND	CONST	RAND	CONST	RAND
AVER	33.24	33.28	36.59	33.12	21.37	23.21
MIN	29.46	29.05	32.42	27.90	17.35	18.05
MAX	39.92	38.55	41.42	37.59	29.01	29.19
STD. DEV.	2.60	2.23	3.05	2.57	2.69	2.87

These data have to be compared with the metric for the reproducibility. We see that the errors are very large, especially for the standard kinematic and isotropic hardening law. The question arises: Are these large errors caused by the numerical values of the parameters or by the structure of the law. It is possible to analyze this question by the selection of the optimal parameters leading to the minimal metric.

The statistics for the optimal parameters for constant amplitude strain is given in Table 3.

TABLE 3. The statistics of the metric  $\Theta_k^{(i)}$  for the optimal parameters.

	a	b	c	d
AVER	32.37	30.28	13.37	11.24
MIN	26.36	24.35	10.10	8.68
MAX	39.02	36.36	18.47	15.10
STD. DEV.	3.35	3.71	1.96	1.53

We observe that the kinematic and isotropic hardening laws are not acceptable because of the structure of the law and not because of the numerical values of the parameters. The Chaboche law is better, especially when the optimal parameters are used. The determination of all 6 parameters from the available published data was very heuristic. Nevertheless, in comparison to the reproducibility, this law is a poor characterization for the optimal parameters. Obviously, the quality of the constitutive law could be still poorer if some other validation problems, especially in higher dimensions, were considered.

**Remarks 1.** In [8], many more results are presented. For example, the statistics of the values of the optimal parameters are given for each of the constitutive laws. These values are reasonably stable (of course, the modulus of plasticity has a much larger spread than the modulus of elasticity).

2. The experiments determine the stresses from the given strains. Although every law has its inverse, the prediction for the strains, if stresses are given is much worse. It is interesting that this deterioration is larger for the Chaboche law than the kinematic law, which indicates that the Chaboche law is less robust. This conclusion relates well to the application of the information gap theory [16].  $\square$

We conclude that all the constitutive laws for plasticity in [8], inclusive of the kinematic law which is often used in computational mechanics, have to be rejected and a larger effort must be made to obtain laws for which the accuracy and the reproducibility metric is comparable or the errors are in a reasonable (by the analyst opinion) range.

We note that there is a large uncertainty in the yield stress which is the basic parameter in the plasticity. For example, Table 1 shows its large sensitivity due to manufacturing. In [3], Volume 1, a large dispersion in the yield stress for steel (iron) is reported.

### 6. The Stochastic Heat Conduction Problem

In Section 3.2, we introduced the stationary heat problem (3.5). In real-life predictions, all input data (i.e. the conductivity coefficients and the source term) always contain uncertainties. In contrast to Section 3, we will now assume that the uncertainty is due to completely known variability. This variability will be characterized in a probabilistic way by a known probability field. Then the problem becomes a stochastic PDE problem. We will follow here [15] where details and precise mathematical formulations are given.

**6.1. The stochastic function in the domain  $D$ . The Karhunen-Loeve expansion.** Let  $(\Omega, \mathcal{F}, \mathcal{P})$  be a complete probability space. Here  $\Omega$  is the set of all outcomes,  $\mathcal{F}$  is the  $\sigma$ -algebra and  $\mathcal{P} : \mathcal{F} \rightarrow [0, 1]$  is the probability measure. Let  $a$  be a stochastic function, which is the thermal conductivity coefficient in (3.7)

with the continuous covariance function  $\text{cov}[a]$ . Define the corresponding compact operator  $T_a : L^2(D) \rightarrow L^2(D)$  given by

$$(6.1) \quad (T_a v)(\mathbf{y}) = \int_D \text{cov}[a](\mathbf{x} \cdot \mathbf{y}) v(\mathbf{x}) dx$$

and let  $(\lambda_i, b_i)$  be the eigenpairs of  $T_a v = \lambda v$ . Then the truncated Karhunen-Loeve expansion  $a_N$  is

$$(6.2) \quad a_N(\omega, \mathbf{x}) = E[a](\mathbf{x}) + \sum_{i=1}^N \sqrt{\lambda_i} b_i(\mathbf{x}) Y_i(\omega)$$

where  $Y_i$  are uncorrelated real random variables with mean zero and unit variance. The random variables  $Y_i$  are uniquely determined by

$$Y_i(\omega) = \frac{1}{\sqrt{\lambda_i}} \int_D (a(\omega, \mathbf{x}) - E[a](\mathbf{x})) b_i(\mathbf{x}) dx$$

and

$$\lim_{N \rightarrow \infty} \{ \sup E[a - a_N^2] \} = \lim_{N \rightarrow \infty} \left( \sum_{\ell=N+1}^{\infty} \lambda_\ell b_\ell^2(\mathbf{x}) \right) = 0$$

Hence  $a_N$  in (6.2) with a fixed  $N$  is an approximation of the stochastic function  $a$ . We will assume in addition:

a. the random variables  $Y_i$  are independent and have probability density  $\varrho_i$  so that the joint probability is

$$(6.3) \quad \varrho(\mathbf{y}) = \prod_{i=1}^N \varrho_i(y_i), \quad \mathbf{y} = (y_1, \dots, y_N)$$

b. the images of  $Y_i(\Omega)$  satisfy  $Y_i(\Omega) \subset \Gamma_i \subset (-\gamma, \gamma)$  and denote  $\Gamma = \prod_{i=1}^N \Gamma_i$ . Further, we assume that  $\varrho \geq \alpha > 0$  on  $\Gamma$ .

c. the eigenfunctions  $b_i$  are smooth on  $D$  and are uniformly bounded.

d. the eigenvalues decay as  $\lambda_i = O(\frac{1}{(1+i)^s})^s$  for some  $s > 1$ .

The stochastic function  $a_N$  can now be identified with a function defined on  $\Gamma \times D$ .

$$a_N(\mathbf{y}, \mathbf{x}), \quad \mathbf{y} = (y_1, \dots, y_N) \in \Gamma, \quad \mathbf{x} \in D$$

We will discuss these assumptions below.

**6.2. The formulation of the stochastic problem and its numerical solution.** The classical deterministic formulation was given in (3.7). Its weak form reads. Find  $u \in H_0^1(D)$  such that

$$(6.4) \quad \int_D a \nabla u \cdot \nabla v \, d\mathbf{x} = \int_D f v \, d\mathbf{x}, \quad \forall v \in H_0^1(\Omega)$$

and the quantity of interest  $Q$  (for example  $Q = \frac{1}{|\omega|} \int_\omega u \, dx$ ). The coercivity assumption

$$(6.5) \quad 0 < a_0 \leq a(\mathbf{x}) \leq a_1 < \infty$$

is essential for the existence and uniqueness of the solution.

In [15] (see also for example [14] and [22] and references therein) it was shown that the stochastic formulation is: Find  $u(\mathbf{y}, \mathbf{x}) \in H = L^2(\Gamma) \times H_0^1(D)$ , which satisfies

$$(6.6) \quad \int_D \int_\Gamma \varrho(\mathbf{y}) a_N(\mathbf{y}, \mathbf{x}) \nabla_x u(\mathbf{y}, \mathbf{x}) \nabla_x v(\mathbf{y}, \mathbf{x}) d\mathbf{x} d\mathbf{y} = \int_D \int_\Gamma f(\mathbf{x}) \varrho(\mathbf{y}) v(\mathbf{y}, \mathbf{x}) d\mathbf{x} d\mathbf{y} \quad \forall v(\mathbf{y}, \mathbf{x}) \in H$$

and find the quantity of interest  $Q$  (for example  $Q = \frac{1}{|S|} \int_\Gamma (\int_S u(\mathbf{y}, \mathbf{x}) d\mathbf{x}) \varrho(\mathbf{y}) d\mathbf{y}$ ,  $S \subset D$ ).

In addition to the coercivity condition (6.5) we also assume that

$$(6.7) \quad 0 < \bar{a}_0 \leq a_N(\mathbf{y}, \mathbf{x}) \leq \bar{a}_i < \infty, \quad \forall \mathbf{y} \in \Gamma, \mathbf{x} \in D, \forall N$$

For simplicity, we assume that the right hand side  $f$  is a deterministic function. We will comment on this later.

The solution  $u(\mathbf{y}, \mathbf{x})$  which depends on  $N$  exists and is unique and for  $N \rightarrow \infty$  it converges to a limit, which is exact solution of the problem. The form (6.6) suggests immediately the finite element method as one numerical approach to this problem. Most natural is to use tensor product h-p elements. For this case ([14], [15]) *a-priori* error estimates have been proven. Among other results, it was proven that p-version approximation in  $\Gamma$  leads to exponential rates of convergence. This is important because  $\Gamma$  has high dimension. An adaptive procedure for selecting degrees  $p$  for the approximation in  $\Gamma$  and adaptive selection of  $N$  was also presented in [14]. This adaptive procedure is based on a simple *a-posteriori* estimation. An illustrative numerical example is presented in [15].

Because the dimension of  $\Gamma$  can be large, it makes sense to also consider a Monte Carlo approach. In [15], an estimate of the complexities of various numerical procedures is given. In [6], a successive approximation (with guaranteed convergence) approach was studied. Such approaches are effective when the covariance function is small.

So far we have assumed that the right hand side  $f$  is deterministic. If the coefficient  $a$  and the right hand side  $f$  are independent, then the problem splits into two parts, one for stochastic  $a$  and deterministic  $f$ , and the other when  $a$  is deterministic and  $f$  is stochastic. This is usually the case in practice. If  $a$  and  $f$  are correlated, then we can proceed analogously, but the process is more complex.

The second case, when only  $f$  is stochastic, is much simpler, especially if we are interested in only the mean and the covariance function of the solution. The mean is the solution of the prediction problem when the right hand side is the mean of  $f$ . The covariance function  $\text{cov}[u]$  is the solution of a boundary value problem on  $D \times D$  with the covariance function of  $f$  at the right hand side ([5]). For an effective numerical treatment, we refer to [41], [22]. This approach can be generalized for determination of higher probabilistic moments; see [40].

Assumptions a - d, in Section 6.1 can be weakened. This could influence the regularity of the solution and the rate of the convergence. Nevertheless, condition c) is essential. If the covariance function  $\text{cov}[a]$  is not sufficiently smooth, for example when  $\text{cov}[a] = e^{-|x-y|}$ , then it was shown in [6] that for sufficiently large  $N$  coercivity of the bilinear form is always violated with a small but positive probability. It is also violated if the images  $y_i(\Omega)$  are not bounded. Then the solution also does not exist with small but positive probability. Conditions (c) and (d) above are fully determined by the covariance function.

There are many open mathematical problems when the dimension of  $\Gamma$  is large and/or the covariance length is small. The numerical solution can be very expensive and very effective procedures have to be used.

Another significant problem is the determination of the Karhunen-Loeve expansion from experimental results. This problem was studied in [9] when the experiments were created virtually as the realizations of a particular Karhunen-Loeve expansion. The question was how to reconstruct the data in the expansion with a reasonable accuracy. It was seen that any reasonable accuracy of the Karhunen-Loeve expansion needs so many experiments that it is practically unfeasible. Because large sets of experiments need to be done, expert opinions dealing with the ignorance are unavoidable. For example, it is possible to treat all inputs in the Karhunen-Loeve expansion as data with an uncertainty-ignorance, as in Section 3. Approaches such as Bayesian probability will likely have to be used. Without solving this problem, the stochastic approach cannot lead to a reliable prediction.

## 7. Conclusion

We have shown that reliable computer predictions of physical events of interest is a very complex problem. The modeling which has to take into consideration the unavoidable uncertainty is very often the bottleneck of a reliable prediction,

The verification of the numerical treatment (*a posteriori* error estimation) is a necessary but not sufficient process for reliable prediction. Many mathematical problems in CS are open. Without addressing them, CS remain not reach its great potential.

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