1

# Introduction

Engineering decision-making processes increasingly rely on information computed from approximate solutions of mathematical models. Engineering decisions have legal and ethical implications. The standard applied in legal proceedings in civil cases in the United States is to have opinions, recommendations and decisions "based upon a reasonable degree of engineering certainty." Codes of ethics of engineering societies impose higher standards. For example, the Code of Ethics of the Institute of Electrical and Electronics Engineers (IEEE) requires members "to accept responsibility in making engineering decisions consistent with the safety, health, and welfare of the public, and to disclose promptly factors that might endanger the public or the environment" and "to be honest and realistic in stating claims or estimates based on available data."

An important challenge facing the computational engineering community is to establish procedures for creating evidence that will show, with a high degree of certainty, that a mathematical model of some physical reality, formulated for a particular purpose, can in fact represent the physical reality in question with sufficient accuracy to make predictions based on mathematical models useful and justifiable for the purposes of engineering decision-making and the errors in the numerical approximation are sufficiently small. There is a large and rapidly growing body of work on this subject. See, for example, [38a], [68], [52], [51], [99]. The formulation and numerical treatment of mathematical models for use in support of engineering decision-making in the field of solid mechanics is addressed in a document issued by the American Society of Mechanical Engineers (ASME) and adopted by the American National Standards Institute (ANSI) [33]. The Simulation Interoperability Standards Organization (SISO) is another important source of information.

The considerations underlying the selection of mathematical models and methods for the estimation and control of modeling errors and the errors of discretization are the two main topics of this book. In this chapter a brief overview is presented and the basic terminology is introduced.

Introduction to Finite Element Analysis: Formulation, Verification and Validation, First Edition. Barna Szabó and Ivo Babuška. © 2011 John Wiley & Sons, Ltd. Published 2011 by John Wiley & Sons, Ltd.



Figure 1.1 The main elements of numerical simulation and the associated errors.

# **1.1** Numerical simulation

The goal of numerical simulation is to make predictions concerning the response of physical systems to various kinds of excitation and, based on those predictions, make informed decisions. To achieve this goal, mathematical models are defined and the corresponding numerical solutions are computed. Mathematical models should be understood to be idealized representations of reality and should never be confused with the physical reality that they are supposed to represent.

The choice of a mathematical model depends on its intended use: What aspects of physical reality are of interest? What data must be predicted? What accuracy is required? The main elements of numerical simulation and the associated errors are indicated schematically in Figure 1.1.

Some errors are associated with the mathematical model and some errors are associated with its numerical solution. These are called errors of idealization and errors of discretization respectively. For the predictions to be reliable both kinds of errors have to be sufficiently small. The errors of idealization are also called modeling errors. Conceptualization is a process by which a mathematical model is formulated. Discretization is a process by which the exact solution of the mathematical model is approximated. Extraction is a process by which the data of interest are computed from the approximate solution. Some authors refer to the data of interest by the term "system response quantities" (SRQs).

# **1.1.1 Conceptualization**

Mathematical models are operators that transform one set of data, the input, into another set, the output. In solid mechanics, for example, one is typically interested in predicting displacements, strains and stresses, stress intensity factors, limit loads, natural frequencies, etc., given a description of the solution domain, constitutive equations and boundary conditions (loading and constraints). Common to all models are the equations that represent the conservation of momentum (in static problems the equations of equilibrium), the strain–displacement relations and constitutive laws.

The end product of conceptualization is a mathematical model. The definition of a mathematical model involves specification of the following:

 Theoretical formulation. The applicable physical laws, together with certain simplifications, are stated as a mathematical problem in the form of ordinary or partial differential equations, or extremum principles. For example, the classical differential equation for elastic beams is derived from the assumptions of the theory of elasticity supplemented by the assumption that the transverse variation of the longitudinal components of the

NUMERICAL SIMULATION 3

displacement vector can be approximated by a linear function without significantly affecting the data of interest, which are typically the displacements, bending moments, shear forces, natural frequencies, etc.

- 2. Specification of the input data. The input data comprise the following:
  - (a) Data that characterize the solution domain. In engineering practice solution domains are usually constructed by means of computer-aided design (CAD) tools. CAD tools produce idealized representations of real objects. The details of idealization depend on the choice of the CAD tool and the skills and preferences of its operator.
  - (b) Physical properties (elastic moduli, yield stress, coefficients of thermal expansion, thermal conductivities, etc.)
  - (c) Boundary conditions (loads, constraints, prescribed temperatures, etc.)
  - (d) Information or assumptions concerning the reference state and the initial conditions
  - (e) Uncertainties. When some information needed in the formulation of a mathematical model is unknown then the uncertainty is said to be cognitive (also called epistemic). For example, the magnitude and distribution of residual stresses is usually unknown, some physical properties may be unknown, etc. Statistical uncertainties (also called aleatory uncertainties) are always present. Even when the average values of needed physical properties, loading and other data are known, there are statistical variations, possibly very substantial variations, in these data. Consideration of these uncertainties is necessary for proper interpretation of the computed information.

Various methods are available for accounting for uncertainties. The choice of method depends on the quality and reliability of the available information. One such method, known as the Monte Carlo method, is to characterize input data as random variables and use repeated random sampling to compute their effects on the data of interest. If the probability density functions of the input data are sufficiently accurate and sufficiently large samples are taken then a reasonable estimate of the probability distribution of the data of interest can be obtained.

3. Statement of objectives. Definitions of the data of interest and the corresponding permissible error tolerances.

Conceptualization involves the application of expert knowledge, virtual experimentation and calibration.

### Application of expert knowledge

Depending on the intended use of the model and the required accuracy of prediction, various simplifying assumptions are introduced. For example, the assumptions incorporated in the linear theory of elasticity, along with simplifying assumptions concerning the domain and the boundary conditions, are widely used in mechanical and structural engineering applications. In many applications further simplifications are introduced, resulting in beam, plate and shell models, planar models and axisymmetric models, each of which imposes additional restrictions on what boundary conditions can be specified and what data can be computed from the solution.

In the engineering literature the commonly used simplified models are grouped into separate model classes, called theories. For example, various beam, plate and shell theories have been developed. The formulation of these theories typically involves a statement on the assumed mode of deformation (e.g., plane sections remain plane and normal to the mid-surface of a deformed beam), the relationship between the functions that characterize the deformation and the strain tensor (e.g., the strain is proportional to the curvature and the distance from the neutral axis), application of Hooke's law, and statement of the equations of the equilibrium.

In undergraduate engineering curricula each model class is presented as a thing in itself and consequently there is a strong predisposition in the engineering community to view each model class as a separate entity. It is much more useful, however, to view any mathematical model as a special case of a more comprehensive model, rather than a member of a conventionally defined model class. For example, the usual beam, plate and shell models are special cases of a model based on the three-dimensional linear theory of elasticity, which in turn is a special case of a large family of models based on the equations of continuum mechanics that account for a variety of hyperelastic, elasto-plastic and other material laws, large deformation, contact, etc. This is the hierarchic view of mathematical models.

Given the rich variety of choices, model selection for particular applications is a non-trivial problem. The goal of conceptualization is to identify the simplest mathematical model that can provide predictions of the data of interest within a specified range of accuracy.

Conceptualization begins with the formulation of a tentative mathematical model based on expert knowledge. We will call this a working model. The term has the same connotation and meaning as the term working hypothesis. Since subjective judgment is involved, the formulation of the initial working model may differ from expert to expert. Nevertheless, assuming that software tools that allow systematic evaluation of mathematical models with respect to clearly defined objectives are available, it should be possible for experts to arrive at a close agreement on the definition of a mathematical model, given its intended use.

### Virtual experimentation

Model selection involves systematic evaluation of the effects of various modeling assumptions on the data of interest and the sensitivity of the data of interest to uncertainties in the input data. This is done through a process called virtual experimentation.

For example, in solid mechanics one usually begins with a working model based on the linear theory of elasticity. The implied assumptions are that the strain is much smaller than unity, the stress is proportional to the strain, the displacements are so small that equilibrium equations written with respect to the undeformed configuration hold in the deformed configuration also, and the boundary conditions are independent of the displacement function. Once a verified solution is available, it is possible to examine the stress field and determine whether the stress exceeded the proportional limit of the material and whether this affects the data of interest significantly. Similarly, the effects of large deformation on the data of interest can be evaluated. Furthermore, it is possible to test the sensitivity of the data of interest to changes in boundary conditions. Virtual experimentation provides valuable information on the influence of various modeling assumptions on the data of interest.

### Calibration

In the process of conceptualization there may be indications that the data of interest are sensitive functions to certain parameters that characterize material behavior or boundary conditions. If those parameters are not available then calibration experiments must be performed

for the purpose of determining the needed parameters. In calibration the mathematical model is assumed to be correct and the parameters that characterize the model are selected such that the measured response matches the predicted response.

**Example 1.1.1** If the goal of computation is to predict the number of load cycles that cause fatigue failure in a metal part then one or more empirical models must be chosen that require as input stress or strain amplitudes and material parameters. One of the widely used models for the prediction of fatigue life in low-cycle fatigue is the general strain–life model:

$$\epsilon_a = \frac{\bar{\sigma}_f}{E} (2N)^b + \bar{\epsilon}_f (2N)^c \tag{1.1}$$

where  $\epsilon_a$  is the strain amplitude, N is the number of cycles to failure, E is the modulus of elasticity,  $\bar{\sigma}_f$  is the fatigue strength coefficient, b is the fatigue strength exponent,  $\bar{\epsilon}_f$  is the fatigue ductility coefficient and c is the fatigue ductility exponent. The parameters E,  $\bar{\sigma}_f$ , b,  $\bar{\epsilon}_f$  and c are determined through calibration experiments. See, for example, [76]. Several variants of this model are in use. Standard procedures have been established for calibration experiments for metal fatigue.<sup>1</sup>

# 1.1.2 Validation

Validation is a process by which the predictive capabilities of a mathematical model are tested against experimental data. We will be concerned primarily with problems in solid mechanics for which the predictions can be tested through experiments especially designed for that purpose. This is a very large class of problems that includes all mathematical models designed for the prediction of the performance of mass-produced items. There are other important problems, such as the effects of earthquakes and other natural disasters, unique design problems, such as dams, siting of nuclear power plants and the like, for which the predictions based on mathematical models cannot be tested at full scale. In such cases the models are analyzed a posteriori and modified in the light of new information collected following an incident.

Associated with each mathematical model is a modeling error (illustrated schematically in Figure 1.1). Therefore it is necessary to have a process for testing the predictive capabilities of mathematical models. This process, called validation. is illustrated schematically in Figure 1.2.



Figure 1.2 Validation.

<sup>&</sup>lt;sup>1</sup> See, for example, the International Organization for Standardization ISO 12106:2003 and ISO 12107:2003.

For a validation experiment one or more metrics and the corresponding criteria are defined. If the predictions meet the criteria then the model is said to have passed the validation test, otherwise the model is rejected.

In large projects, such as the development of an aircraft, a series of validation experiments are performed starting with coupon tests for the determination of physical properties and failure criteria, then progressing to sub-components, components, parts, sub-assemblies and finally the entire assembly. The cost of experiments increases with complexity and hence the number of experiments decreases with complexity. The goal is to develop sufficiently reliable predictive capabilities such that the outcome of experiments involving sub-assemblies and assemblies will confirm the predictions. Finding problems late in the production cycle is generally very costly.

In evaluating the results of validation experiments it is important to bear in mind the limitations and uncertainties associated with the available information concerning the physical systems being modeled:

- 1. The solution domain is usually assumed to correspond to design specifications ("the blueprint"). In reality, parts, sub-assemblies and assemblies deviate from their specifications and the degree of deviation may not be known, or would be difficult to incorporate into a mathematical model.
- 2. For many materials the constitutive laws are known imperfectly and only in some average sense and within a narrow range of strain, strain rate, temperature and over a short time interval of loading.
- 3. The boundary conditions, other than stress-free boundary conditions, are not known with a high degree of precision, even under carefully controlled experimental conditions. The reason for this is that the loading and constraints typically involve mechanical contact which depends on the compliances of the structures that impose the load and constraints (e.g., testing machine, milling machine, assembly rig, etc.) and the physical properties of the contacting surfaces. In other words, the boundary conditions represent the influence of the environment on the object being modeled. The needed information is rarely available. Therefore subjective judgment of the analyst in the formulation of boundary conditions is usually unavoidable.
- 4. Due to the history of the material prior to manufacturing the parts that will be assembled into a machine or structure, such as casting, quenching, extrusion, rolling, forging, heat treatment, cold forming, machining and surface treatment residual stresses exist, the magnitude of which can be very substantial. The distribution of residual stress must satisfy the equations of equilibrium and the stress-free boundary conditions but otherwise it is generally unknown. See, for example, [47], [48].
- 5. Information concerning the probability distribution of the data that characterize the problem and their covariance functions is rarely available. In general, uncertainties increase with the complexity of models.

**Remark 1.1.1** More than one mathematical model may have been proposed with identical objectives and it is possible that more than one mathematical model will meet the validation criteria. In that case the simpler model is.

# NUMERICAL SIMULATION 7

**Remark 1.1.2** Due to statistical variability in the data and errors in experimental observations, comparisons between prediction based on a mathematical model and the outcome of physical experiments must be understood in a statistical sense. The theoretical framework for model selection is based on Bayesian analysis.<sup>2</sup> Specifically, denoting a mathematical model by M, the newly acquired data by D and the background information by I, the probability that the model M is a predictor of the data D, given the background information I, can be written in terms of conditional probabilities:

$$\operatorname{Prob}(M|D, I) \approx \operatorname{Prob}(D|M, I) \times \operatorname{Prob}(M|I).$$
(1.2)

In other words, Bayes' theorem relates the probability that a mathematical model is correct, given the measured data D and the background information I, to the probability that the measured data would have been observed if the model were functioning properly. See, for example, [74]. The term Prob(M|I) is called prior probability. It represents expert opinion about the validity of M prior to coming into possession of some new data D. The term Prob(D|M, I) is called the likelihood function. In this view competing mathematical models are assigned probabilities that represent the degree of belief in the reliability of each of the competing models, given the information available prior to acquiring additional information. In light of the new information, obtained by experiments, the prior probability is updated to obtain the term Prob(M|D, I), called the posterior probability. An important and highly relevant aspect of Bayes' theorem is that it provides a framework for improvement of the probability estimate Prob(M|D, I) based on new data.

# 1.1.3 Discretization

The finite element method (FEM) is one of the most powerful and widely used numerical methods for finding approximate solutions to mathematical problems formulated so as to simulate the responses of physical systems to various forms of excitation. It is used in various branches of engineering and science, such as elasticity, heat transfer, fluid dynamics, electromagnetism, acoustics, biomechanics, etc.

In the finite element method the solution domain is subdivided into elements of simple geometrical shape, such as triangles, squares, tetrahedra, hexahedra, and a set of basis functions are constructed such that each basis function is non-zero over a small number of elements only. This is called discretization. Details will be given in the following chapters. The set of all functions that can be written as linear combinations of the basis functions is called the finite element space. The accuracy of the data of interest depends on the finite element space and the method used for computing the data from the finite element solution. Associated with the finite element solution are errors of discretization, as indicated in Figure 1.1.

It is necessary to create finite element spaces such that the data of interest computed from the finite element solution are within acceptable error bounds with respect to their counterparts corresponding to the exact solution of the mathematical model.

The data of interest, such as the maximum displacement, temperature, stress, etc., are computed from the finite element solution  $u_{FE}$ . The data of interest will be denoted by  $\Phi_i(u_{FE})$ , i = 1, ..., n, in the following. The objective is to compute  $\Phi_i(u_{FE})$  and to ensure

P1: OSO JWST055-01 JWST055-Szabo February 16, 2011 7:52 Printer Name: Yet to Come

<sup>&</sup>lt;sup>2</sup> Thomas Bayes (1702–1761).

that the relative errors are within prescribed tolerances:

$$\frac{|\Phi_i(u_{EX}) - \Phi_i(u_{FE})|}{|\Phi_i(u_{EX})|} \le \tau_i \tag{1.3}$$

where  $u_{EX}$  is the exact solution. Of course  $u_{EX}$  is not known in general, but it is known that  $\Phi_i(u_{EX})$  is independent of the finite element space. The error in  $\Phi_i(u_{FE})$  depends on the finite element space and the method used for computing  $\Phi_i(u_{FE})$ . The errors of discretization are controlled through suitable enlargement of the finite element spaces, and by various procedures used for computing  $\Phi_i(u_{FE})$ .

# 1.1.4 Verification

Verification is concerned with verifying that (a) the input data are correct, (b) the computer code is functioning properly and (c) the errors in the data of interest meet necessary conditions to be within permissible tolerances.

Common errors in input are incorrectly entered data, such as mixed units and errors in data entry. Such errors are easily found in a careful review of the input data.

The primary responsibility for ensuring that the code is functioning properly rests with the code developers. However, computer codes tend to have programming errors, especially in their less frequently traversed branches, and the user shares in the responsibility of verifying that the code is functioning properly.

In verification accuracy is understood to be with respect to the exact solution of the mathematical model, not with respect to physical reality. The process of verification of the numerical solution is illustrated schematically in Figure 1.3. The term extraction refers to methods used for computing  $\Phi_i(u_{FE})$ . Details are presented in the following chapters.

**Remark 1.1.3** Verification and validation are possible only when the mathematical model is properly formulated with respect to the goals of computation. For example, in linear elasticity the solution domain must not have sharp re-entrant corners or edges if the goal of computation is to determine the maximum stress. Point constraints and point forces can be used only when certain criteria are met etc. Details are given in the following chapters. Unfortunately, using mathematical models without regard to their limitations is a commonly occurring conceptual error.



**Figure 1.3** Verification of the numerical solution.

# NUMERICAL SIMULATION 9

**Remark 1.1.4** The process illustrated schematically in Figure 1.1 is often referred to as finite element modeling. This term is unfortunate because it mixes two conceptually different aspects of numerical simulation: the definition of a mathematical model and its numerical solution by the finite element method.

# 1.1.5 Decision-making

The goal of numerical simulation is to support various engineering decision-making processes. There is an implied expectation of reliability: one cannot reasonably base decisions on computed information without believing that the information is sufficiently reliable to support those decisions. Demonstration of the reliability of mathematical models used in support of engineering decision-making is an essential part of any modeling effort. In fact, the role of physical testing is to calibrate and validate mathematical models so that a variety of load cases and design alternatives can be evaluated.

In the following we illustrate the importance of the reliability of numerical simulation processes through brief descriptions of four well-documented examples of the consequences of large errors in prediction either because improper mathematical models were used or because large errors occurred in the numerical solution. Additional examples can be found in [61], [62]. Undoubtedly, there are many undocumented instances of substantial loss attributable to errors in predictions based on mathematical models.

**Example 1.1.2** The Tacoma Narrows Bridge, the first suspension bridge across Puget Sound (Washington State, USA), collapsed on November 7, 1940, four months after its opening. Wind blowing at 68 km/h caused sufficiently large oscillations in the 853 m main span to collapse the span.

Until that time bridges were designed on the basis of equivalent static forces. The possibility that relatively small periodic aerodynamic forces (the effects of Kármán vortices)<sup>3</sup> may become significant was not considered. The Kármán vortices were first analyzed in 1911 and the results were presented in the Göttingen Academy in the same year.<sup>4</sup> The designers were either unaware of those results or did not see their relevance to the Tacoma Narrows Bridge, the failure of which was caused by insufficient torsional stiffness to resist the periodic excitation induced by Kármán vortices.

**Example 1.1.3** The roof of the Hartford Civic Center Arena collapsed on January 18, 1978. The roof structure, measuring 91.4 by 109.7 m (300 by 360 ft), was a space frame, an innovative design at that time. It was analyzed using a mathematical model that accounted for linear response only. Furthermore, the connection details were greatly simplified in the model. In linear elastostatic analysis it is assumed that the deformation of a structure is negligibly small and hence it is sufficient to satisfy the equations of equilibrium in the undeformed configuration.

The roof frame was assembled on the ground. Once the roof was lifted into its final position, its deflection was measured to be twice of what was predicted by the mathematical model:

<sup>&</sup>lt;sup>3</sup> Theodore von Kármán (1881–1963).

<sup>&</sup>lt;sup>4</sup> Von Kármán, Th. and Edson, L., *The Wind and Beyond: Theodore von Kármán, Pioneer in Aviation and Pathfinder in Space*, Little, Brown, Boston, MA, 1967, pp. 211–215.

When notified of this condition, the engineers expressed no concern, explaining that such discrepancies had to be expected in view of the simplifying assumptions of the theoretical calculation.<sup>5</sup>

Subsequent investigation identified that reliance on an oversimplified model that did not represent the connection details properly and failed to account for geometric nonlinearities was the primary cause of failure.

**Example 1.1.4** The Vaiont Dam, one of the highest dams in the world (262 m), was completed in the Dolomite Region of the Italian Alps, 100 km north of Venice, in 1961. On October 9, 1963, after heavy rains, a massive landslide into the reservoir caused a large wave that overtopped the dam by up to 245 m and swept into the valley below, resulting in the loss of an estimated 2000 lives.<sup>6</sup> The courts found that, due to the *predictability* of the landslide, three engineers were criminally responsible for the disaster. The dam withstood the overload caused by the wave. This incident serves as an example of a full scale test of a major structure caused by an unexpected event.

**Example 1.1.5** The consequences of large errors of discretization are exemplified by the Sleipner accident. The gravity base structure (GBS) of the Sleipner A offshore platform, made of reinforced concrete, sank during ballast test operations in Gandsfjorden, south of Stavenger, Norway, on August 23, 1991. The economic loss was estimated to be 700 million dollars.

The main function of the GBS was to support a platform weighing 56 000 tons. The GBS consisted of 24 caisson cells with a base area of  $16\,000\,\text{m}^2$ . Four cells were elongated to form shafts designed to support the platform. The total concrete volume of the GBS was 75 000 m<sup>3</sup>. The accident occurred as the GBS was being lowered to a depth of approximately 99 m. Failure first occurred in two triangular cells, called tri-cells, next to one of the shafts. When the GBS hit the sea bed, seismic events measuring 3 on the Richter scale were recorded in the Stavenger area.<sup>7</sup>

There is general agreement among the investigators that the accident was caused by large errors in the finite element analysis, the goal of which was to estimate the requirements for reinforcement of the concrete cells by steel bars:

The global finite element analysis gave a 47% underestimation of the shear forces in the tri-cell walls. This error was caused by the use of a coarse finite element mesh with some skewed elements used for analysis of the tri-cell walls.<sup>8</sup>

<sup>&</sup>lt;sup>5</sup> Levy, M. and Salvadori, M., Why Buildings Fall Down: How Structures Fail, W. W. Norton, New York, 2002.
<sup>6</sup> See, for example, Hendron, A. J. and Patten, F. D., The Vaiont Slide. US Corps of Engineers Technical Report GL-85-8 (1985).

<sup>&</sup>lt;sup>7</sup> Jacobsen, B., The loss of the Sleipner A Platform, *Proceedings of the 2nd International Offshore and Polar Engineering Conference*, International Society of Offshore and Polar Engineers, Vol. 1, 1992.

<sup>&</sup>lt;sup>8</sup> Rettedal, W. K., Gudmestad, O. T. and Aarum, T., Design of concrete platforms after Sleipner A-1 sinking, *Proceedings of the 12th International Conference on Offshore Mechanics and Arctic Engineering*, Vol. 1, Offshore Technology, pp. 309–310, ASME, 1993.

### WHY IS NUMERICAL ACCURACY IMPORTANT?

A check of the global response analysis revealed serious inaccuracies in the interpretation of results from finite element analyses giving a shear force in a critical section of the cell wall that was less than 60% of the correct value.<sup>9</sup>

#### 1.2 Why is numerical accuracy important?

A number of difficulties associated with accurate representation of a real physical system by mathematical means were noted in Section 1.1.2. Given these difficulties, it may seem reasonable to ask: "If we do not know the input data with sufficient accuracy, then why should we be concerned with the accuracy of the numerical solution?" In answering this question we consider two important areas of application of mathematical models: the application of design rules and the formulation of design rules. It is shown in the following that both require estimation and control of the numerical accuracy.

#### 1.2.1 **Application of design rules**

Design and design certification involve application of existing design rules, established by various codes, regulations and guidelines. The design rules are typically stated in the form of required minimum factors of safety:

$$FS := \frac{\Phi_{\lim}}{\Phi_{\max}(u_{EX})} \ge (FS)_{\text{design}}$$
(1.4)

where FS is the realized factor of safety,  $\Phi_{\text{lim}} > 0$  is the limiting (not to exceed) value of some entity (such as maximum bending moment, maximum stress, etc.),  $\Phi_{max}(u_{EX}) > 0$  is the exact value of the same entity corresponding to the exact solution of the mathematical model and  $(FS)_{\text{design}}$  is the minimum value of the factor of safety specified by the applicable design rules. It is the designer's responsibility to ensure that the applicable design rules are followed.

We will denote by  $\Phi_{\max}(u_{FE})$  the value of  $\Phi_{\max}$  computed from the finite element solution. Let us suppose that, due to numerical errors, it is possible to guarantee only that the relative error is not greater than  $\tau$ :

$$\frac{|\Phi_{\max}(u_{EX}) - \Phi_{\max}(u_{FE})|}{\Phi_{\max}(u_{EX})} \le \tau, \quad 0 \le \tau < 1;$$

$$(1.5)$$

in other words,  $\Phi_{\max}(u_{FE})$  may underestimate  $\Phi_{\max}(u_{EX})$  by 100 $\tau$ %. Therefore we have

$$\Phi_{\max}(u_{EX}) \le \frac{1}{(1-\tau)} \Phi_{\max}(u_{FE}).$$
(1.6)

On substituting this expression into Equation (1.4), we obtain

$$\frac{\Phi_{\lim}}{\Phi_{\max}(u_{FE})} \ge \frac{(FS)_{\text{design}}}{1-\tau}.$$
(1.7)

11

<sup>&</sup>lt;sup>9</sup> Holand, I., The Sleipner accident, in From Finite Elements to the Troll Platform - Ivar Holand 70th Anniversary, K. Bell, editor, The Norwegian Institute of Technology, Trondheim, pp. 157-168, 1994.

On comparing Equation (1.7) with Equation (1.4) it is seen that, to compensate for numerical errors in the computation of  $\Phi_{\max}(u_{FE})$ , it is necessary to increase the required factor of safety to  $(FS)_{\text{design}}/(1-\tau)$ . For example, if the accuracy of  $\Phi_{\max}(u_{FE})$  can be guaranteed to 20% (i.e.,  $\tau = 0.20$ ) then  $(FS)_{\text{design}}$  must be increased by 25%. Since  $(FS)_{\text{design}}$  was chosen conservatively to account for the uncertainties, the economic penalties associated with using an increased factor of safety generally far outweigh the costs associated with guaranteeing the accuracy of the data of interest to within a small relative error (say 5%).

Application of design rules is a task of verification, that is, verification that the correct data are used, the computer code is functioning properly and the tolerance  $\tau$  in Equation (1.5) is sufficiently small.

**Remark 1.2.1** In aerospace engineering the design requirements are stated in terms of minimum acceptable margins of safety (*MS*). By definition, MS = FS - 1.

**Remark 1.2.2** The Federal Aviation Regulations (FAR), issued by the Federal Aviation Administration of the US Department of Transportation, state in Sec. 25.303 that "a factor of safety of 1.5 must be applied to the prescribed limit load."

Economic considerations dictate that the realized factor of safety should not be much larger than  $(FS)_{design}$ . This is especially true in aerospace engineering where avoidance of weight penalties makes it necessary to ensure that the realized factors of safety are reasonably close to the mandated factors of safety.

**Example 1.2.1** The yield strength in shear of hot rolled 0.2% carbon steel is 165 MPa and the usual factor of safety for static loads is 1.65 (so that the allowable maximum shear stress is 100 MPa).<sup>10</sup> If the numerical computations could underestimate the maximum shear stress by as much as 20% then the factor of safety would have to be increased to 2.06, that is, the allowable maximum value would be reduced to 80 MPa.

# **1.2.2** Formulation of design rules

The responsibility for formulating design rules rests with committees of experts appointed by professional societies and regulatory bodies. Some of the design rules have been evolving for a long time while others are still in their early stages of development. For example, the ASME Boiler and Pressure Vessel Code dates back to 1914. It has been adopted in part or in its entirety by all 50 states of the United States. The code is being updated by the Boiler and Pressure Committee which meets regularly to consider requests for interpretations, revision, and to develop new rules. On the other hand, design rules for structural components of aircraft made of laminated composites are in their early stages of development

The formulation and revision of design rules are applications of the process of validation discussed in Section 1.1.2 and schematically illustrated in Figure 1.2 in the following sense. The object of design is the physical reality. The mathematical model is the collection of physical laws that experts consider relevant to decision-making. The formulas and rules are, respectively, the metrics and criteria used in the prediction that the object of design will

<sup>&</sup>lt;sup>10</sup> See, for example, Popov, E. P., *Engineering Mechanics of Solids*, 2nd edition, Prentice Hall, Upper Saddle River, NJ, 1998.

### WHY IS NUMERICAL ACCURACY IMPORTANT? 13

function as intended when the stated criteria are satisfied. In light of new experience, the model, metrics and criteria are revised.

Formulation of design rules involves definition of certain entities  $\Phi_k$  (k = 1, 2, ...), such as the maximum principal stress, some specific combinations of stress and strain components, etc., that characterize failure and the corresponding limiting values. In the following the subscript k will be dropped and the discussion will be concerned with a generic design rule, that is, the determination of  $\Phi_{\text{lim}}$  and evaluation of the associated uncertainties. The factor of safety is determined on the basis of assessment of uncertainties and consideration of the consequences of failure.

Suppose that a mathematical model predicts that failure will occur when  $\Phi$  reaches its critical value  $\Phi_{lim}$ . First, a set of calibration experiments have to be performed with the objective to determine  $\Phi_{lim}$ . Second, another set of experiments have to be conducted to test whether failure can be predicted on the basis of  $\Phi_{lim}$ . These are validation experiments. In general  $\Phi$  cannot be observed directly, therefore it must be inferred from correlations between computed data and experimental observations.

Let  $Y_{ij}$  be the *i*th ideal observation of the *j*th experiment and let  $\phi_i(u_{EX}^{(j)})$  be the corresponding functional<sup>11</sup> computed from the exact solution  $u_{EX}^{(j)}$  so that if there were no experimental errors and the mathematical model were correct then we would have

$$Y_{ij} - \phi_i(u_{EX}^{(j)}) = 0.$$

Due to experimental errors we actually observe  $y_{ij}$  and compare it with  $\phi_i(u_{FE}^{(j)})$ , the finite element approximation to  $\phi_i(u_{EX}^{(j)})$ . Let us write

$$Y_{ij} = y_{ij} \pm e_{ij}^{\exp}$$

and

$$\phi_i(u_{EX}^{(j)}) = \phi_i(u_{FE}^{(j)}) \pm e_{ij}^{\text{fea}}$$

where  $e_{ii}^{exp}$  (resp.  $e_{ii}^{fea}$ ) is the experimental (resp. approximation) error. Then

$$y_{ij} - \phi_i(u_{FE}^{(j)}) = Y_{ij} \mp e_{ij}^{\exp} - \phi_i(u_{EX}^{(j)}) \pm e_{ij}^{\text{fea}}.$$

Using the triangle inequality, we have

$$\underbrace{|y_{ij} - \phi_i(u_{FE}^{(j)})|}_{\text{apparent error}} \leq \underbrace{|Y_{ij} - \phi_i(u_{EX}^{(j)})|}_{\text{true error}} + |e_{ij}^{\text{exp}}| + |e_{ij}^{\text{fea}}|.$$
(1.8)

This result shows that in testing a mathematical model it is essential to have both the experimental errors and the errors of discretization under control, otherwise it will not be possible to know whether the apparent error is due to an error in the hypothesis, errors in the numerical approximation, or errors in the experiment. Furthermore, means for the estimation

<sup>&</sup>lt;sup>11</sup> A functional is a real number defined on a space of functions. In the present context a functional is a real number computed from the exact solution or the finite element solution.

and control of discretization errors, in terms of the data of interest, must be provided by the computer code.

The aim of experiments needs to include the development of reliable statistical information on the basis of which the factor of safety is established.

# **1.3** Chapter summary

The principal aim of this book is to present the theoretical and practical considerations relevant to (a) the validation of mathematical models and (b) verification of the data of interest computed from finite element solutions. Some fundamental concepts and basic terminology were introduced, as follows.

## Mathematical model

A mathematical representation of a physical system or process intended for predicting some set of responses is called a mathematical model. It transforms one set of data, the input, into another set, the output.

### Conceptualization

Conceptualization is a process by which a mathematical model is defined, for a particular application. Conceptualization involves (a) application of expert knowledge, (b) virtual experimentation and (c) calibration.

# Discretization

Discretization is a process by which a mathematical problem is formulated that can be solved on digital computers. The solution approximates the exact solution of a given mathematical model.

# Validation

Validation is a process by which the predictive capabilities of mathematical models are tested. Ideally, experiments are conducted especially to test whether a mathematical model meets necessary conditions for acceptance from the perspective of its intended use. If the predictions based on the model are not sufficiently close to the outcome of physical experiments then the model is rejected. The quality of predictions is evaluated on the basis of one or more metrics and the corresponding criteria, formulated prior to the execution of validation experiments. Of course, the comparisons must take into account uncertainties in the model parameters, the accuracy of numerical solutions and errors in the experiments.

It is generally feasible to perform full scale validation experiments for mass-produced items. For one-of-a-kind objects, such as dams, bridges, buildings, etc., it is not feasible to perform full scale validation experiments. In such cases the model is analyzed a posteriori in light of new information collected following an incident.

# CHAPTER SUMMARY 15

# Verification

Verification is a process by which it is ascertained that the data of interest computed from the approximate solution meet the necessary conditions for acceptance. Verification is understood in relation to the exact solution of a mathematical model, not in relation to the physical reality that the mathematical model is supposed to represent.

# Uncertainties

It is important to distinguish between statistical (aleatory) and cognitive (epistemic) uncertainties. In the process of calibration the mathematical model is assumed to be correct and the parameters that characterize the model are selected such that the measured response matches the predicted response. Consequently aleatory and epistemic uncertainties are unavoidably mixed. Epistemic uncertainties can be reduced when the predictive capabilities of alternative models are systematically tested and revised as new experimental information becomes available. This involves reinterpretation of the available experimental data with reference to the revised model. P1: OSO JWST055-01 JWST055-Szabo February 16, 2011 7:52 Printer Name: Yet to Come