Selected References on Reliability in Numerical Simulation

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The problem of reliability in numerical simulation based on the finite element method (FEM) has been addressed in a number of papers. The purpose of this Technical Brief is to present a brief survey of what the writer considers to be some of the key contributions to this important subject in the field of solid mechanics.

The notion of reliability

The results of numerical simulation cannot be considered reliable unless it can be shown that the mathematical model properly accounts for all physical attributes that affect the data of interest in the system being modeled and the data of interest computed from the approximate solution meet necessary conditions to be within acceptable tolerances.

In the following we denote the exact solution of the mathematical model by $\mathbf{u}_{\mathrm{EX}}$ and the finite element solution by $\mathbf{u}_{\mathrm{FE}}$, which is understood to be an approximation to $\mathbf{u}_{\mathrm{EX}}$. We are interested in computing some data from the finite element solution $\Phi_i(\mathbf{u}_{\mathrm{FE}})$, $i=1,2,\ldots$ and would like to know whether $\Phi_i(\mathbf{u}_{\mathrm{FE}})$ are sufficiently close to $\Phi_i(\mathbf{u}_{\mathrm{EX}})$. The errors $|\Phi_i(\mathbf{u}_{\mathrm{EX}}) - \Phi_i(\mathbf{u}_{\mathrm{FE}})|$, called *errors of discretization*, depend on the finite element mesh, the polynomial degree of the elements, the mapping functions and the method by which $\Phi_i(\mathbf{u}_{\mathrm{FE}})$ were computed, that is, *choices made by the analyst*. The available choices depend on particular software implementations, nevertheless estimation and control of discretization errors are among the key responsibilities of analysts.

We denote the data of interest associated with the physical system and process that the mathematical model is supposed to represent by Φ_i^*. The errors $|\Phi_i^* - \Phi_i(\mathbf{u}_{\mathrm{EX}})|$ are associated with the choice of the mathematical model and are called the *errors of idealization.* Some of the data of interest can be observed in physical experiments, most cannot. If we compare the predictions based on a mathematical model with experimental data then we are interested in the errors of idealization. However, since we generally do not know $\mathbf{u}_{\mathrm{EX}}$, we compute $|\Phi_i^* - \Phi_i(\mathbf{u}_{\mathrm{FE}})|$. Clearly, $|\Phi_i^* - \Phi_i(\mathbf{u}_{\mathrm{FE}})|$ cannot be a close approximation to $|\Phi_i^* - \Phi_i(\mathbf{u}_{\mathrm{EX}})|$ unless it can be shown that $|\Phi_i(\mathbf{u}_{\mathrm{FE}}) - \Phi_i(\mathbf{u}_{\mathrm{EX}})|$ is small (not larger than the experimental error associated with the measurement of Φ_i^*). In other words, the model can be *validated* only if it is first *verified* that the error in the numerical solution is small. The subjects of verification and validation (V&V) are discussed in two ESRD technical briefs [1], [2]. The fundamental importance of V&V in computational engineering and the associated challenges are highlighted in [3], [4]. Some of the key references that address various aspects of V&V are listed in the following.

References on a posteriori error estimation

The errors of discretization $|\Phi_i(\mathbf{u}_{\mathrm{EX}}) - \Phi_i(\mathbf{u}_{\mathrm{FE}})|$ are estimated by techniques of a posteriori error estimation. From the theoretical point of view, techniques of a posteriori error estimation are well developed for the h-version of FEM (h-FEM); reference [5] is a comprehensive treatment of this subject. These techniques are not available to users of commercial h-FEM software products however, with the possible exception of error estimation in energy norm for linear elasticity and similar problems, typically based on some variant of the Zienkiewicz-Zhu estimator (see, for example, [5]). Since generally the error in energy norm is not an indicator of the error in the data of interest, it is very difficult to estimate and control the errors of discretization in terms of the data of interest by means of the currently available commercial implementations of h-FEM.

Implementations of the p-version of FEM (p-FEM) make it convenient to obtain converging sequences of finite element solutions and hence *feedback information* on the quality of approximation: Since $\Phi_i(\mathbf{u}_{\mathrm{EX}})$ is independent of the mesh and polynomial degree, the error $|\Phi_i(\mathbf{u}_{\mathrm{EX}}) - \Phi_i(\mathbf{u}_{\mathrm{FE}})|$ cannot be small unless $\Phi_i(\mathbf{u}_{\mathrm{FE}})$ is also substantially independent of the mesh and the polynomial degree. This is a necessary condition that can be easily tested by means of the p-FEM.

The theoretical basis and aspects of implementation of p-FEM are available in [6], [7]. Using feedback information for the estimation and control of both the errors of discretization and the errors of idealization is discussed in [8], [9]. The convergence of stress maxima in p-FEM is addressed in [10]. Superconvergent procedures for the computation of stress and flux intensity factors are described in [11], [12], [13].

References on the selection of mathematical models

Selection of mathematical models is based on experience, computational trials and physical experiments. Analysts usually start with simple models and gradually refine them until they are satisfied that all essential attributes of the physical system have been taken into account. Implied is a hierarchic view of mathematical models; each model is viewed as a special case of a more comprehensive model. As the complexity of models increase, more descriptive information of the physical system is needed. Proper model selection and proper definition of input data are the great challenges of computational engineering. The purpose of validation is to ensure that the mathematical model used for predicting the response of a physical system meets necessary conditions for accounting for all of its essential attributes.

Hierarchic models for structural plates and shells have been described in [6] [7], [14]. Application of the hierarchic concept to laminated plates are presented in [15] and to shells in [16]. Procedures for verification and validation of working models for shells are described in [17].

Application of p-FEM to the solution of elastic-plastic problems is described in [18], [19], [20]. Reference [19] presents comparisons between the performances of h-FEM and p-FEM on the basis of a benchmark problem. Application of the p-FEM to geometrically nonlinear problems is described in [21], [22] and in combination with hyperelasticity in [23]. The application of p-FEM to the solution of problems involving elastic contact is described in [24]. The problem of modeling structural connections, involving contact and material non-linearity, is discussed and illustrated by examples in [25].

These nonlinear capabilities, combined with feedback information from converging sequences of finite element solutions, are essential for the identification of models that pass validations tests.

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