Mechanics-based verification method - application to computational models

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MECHANICS-BASED VERIFICATION METHOD - APPLICATION TO COMPUTATIONAL MODELS

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Summary This work introduces a general procedure to control (globally or in a goal-oriented way) the accuracy of simulation models used in Computational Mechanics. This procedure, which is based on the Constitutive Relation Error, provides for guaranteed and high quality bounds on the discretization error for a large panel of Mechanical Engineering models solved by approximate methods. It also enables to assess modeling errors which are generated in model reduction methods using reduced bases.

INTRODUCTION

Numerical simulations are nowadays a common tool in mechanical engineering and design. Nevertheless, in order to be fully reliable, this tool requires a permanent control of the numerical models it involves; this is a major scientific concern known as model verification. For more than thirty years, this research topic has been extensively addressed and gave birth to several performing methods, in particular for the assessment of the global discretization error. More recently, research concentrated on *goal-oriented error estimation*, that is estimation of the error on specific outputs of interest which are relevant for design purposes. Several techniques were proposed for goal-oriented error estimation applied to linear and nonlinear problems, but few of them really provide for strict error bounds which is a drawback for robust design.

A general verification framework has been introduced in the last years to address robust verification of simulation models arising from the finite element method [1]. It is based on the Constitutive Relation Error (CRE), which is a powerful and mechanically sound tool [2], as well as adjoint-based techniques devoted to the quantity of interest under study [3]. Several works illustrated the performances of this method for controlling discretization parameters when dealing with (visco-)elasticity problems, fracture mechanics problems solved with XFEM, transient dynamics problems, or nonlinear (visco-)plasticity problems. Moreover, the verification method has also been extended to take into account modeling errors encountered in model reduction methods, especially in the Proper Generalized Decomposition (PGD) which is increasingly used nowadays [4].

We give below the main ideas of the proposed approach. Technical details and implementation purposes will be given during the presentation, and performances for error control will be shown on several 3D industrial applications.

THE CONSTITUTIVE RELATION ERROR

The CRE is a very general concept for model verification [2], providing for guaranteed bounds on the discretization error. As a simple illustration, let us consider a linear elasticity problem, with displacement-stress solution $(\mathbf{u}, \sigma)$, and let us assume it is solved using the finite element method leading to the approximate solution $(\mathbf{u}_h, \sigma_h)$. The use of CRE first requires the construction of an admissible pair $(\hat{\mathbf{u}}_h, \hat{\sigma}_h)$ i.e. a displacement field $\hat{\mathbf{u}}_h$ that verifies kinematics constraints of the problem, and a stress field $\hat{\sigma}_h$ that verifies balance equations. This construction is in practice performed from a post-processing of $(\mathbf{u}_h, \sigma_h)$ (see [5]). The CRE is then defined as:

$$E_{CRE}(\hat{\mathbf{u}}_h, \hat{\sigma}_h) = ||\hat{\sigma}_h - \mathbf{K}\varepsilon(\hat{\mathbf{u}}_h)|| \tag{1}$$

i.e. as a global measure (in energetic norm) of how the admissible pair $(\hat{\mathbf{u}}_h, \hat{\sigma}_h)$ fails at verifying the constitutive relation (here Hooke's law $\sigma = \mathbf{K}\varepsilon(\mathbf{u})$). It is then easy to show (Prager-Synge's equality) that $E_{CRE}(\hat{\mathbf{u}}_h, \hat{\sigma}_h)$ is an upper bound on the discretization error; local error indicators can also be derived for mesh adaptation (see Fig. 1).

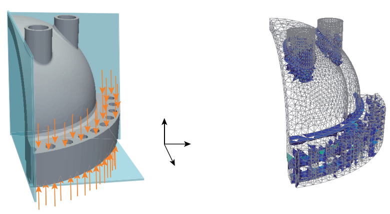

Figure 1. Use of the CRE method on a 3D structure: mechanical model (left) and discretization error distribution (right).

The CRE concept and its properties can be extended to time-dependent and nonlinear problems, E_{CRE} being in that case constructed from dissipative terms (measure of the error on evolution laws) [2].

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GOAL-ORIENTED ERROR ESTIMATION

In many cases, numerical simulations do not aim at predicting the whole solution of the physical phenomenon under study, but only some specific aspects, i.e. local features (maximal displacement, stress intensity factors, etc...) referred as quantities of interest (denoted $I(\mathbf{u})$) and primarily used for design purposes. It makes therefore sense to control only parameters which are influent for these quantities of interest, leading to a goal-oriented verification procedure. For that objective, a classical approach leans on the solution, denoted $(\tilde{\mathbf{u}}, \tilde{\sigma})$, of an adjoint problem [3]. The use of the CRE concept on the adjoint problem as well (with measure $E_{CRE}(\hat{\tilde{\mathbf{u}}}_h, \hat{\tilde{\sigma}}_h)$) provides for a guaranteed bounding of the type:

$$|I(\mathbf{u}) - I(\mathbf{u}_h) - I_{hh}| \leq E_{CRE}(\hat{\mathbf{u}}_h, \hat{\sigma}_h) \times E_{CRE}(\hat{\tilde{\mathbf{u}}}_h, \hat{\tilde{\sigma}}_h) \tag{2}$$

where I_{hh} is a computable correcting term. Let us note that no Galerkin orthogonality property is used to obtain (2), so that independent meshes can be used to solve reference and adjoint problems.

In recent works, a non-intrusive approach was proposed to solve the adjoint problem, which provides for accurate errors bounds on I at low cost and enables to consider the case of pointwise quantities of interest in time and space. This attractive approach is based on a local enrichment using handbook techniques, i.e. searching the adjoint displacement field under the form $\tilde{\mathbf{u}} = \tilde{\mathbf{u}}^{hand}\Phi + \tilde{\mathbf{u}}^{res}$ where:

- $\tilde{\mathbf{u}}^{hand}$ is an enrichment function that is picked among (generalized) Green's solutions in a (semi-)infinite domain. It is obtained analytically [6], when possible, or is computed numerically (see Fig. 2 for a 3D example);
- Φ is a weighting function, with bounded support, so that the enrichment is introduced locally. It is in practice constructed by means of the partition of unity defined by linear shape functions;
- $\tilde{\mathbf{u}}^{res}$ is a residual term that enables to verify boundary conditions of the adjoint problem.

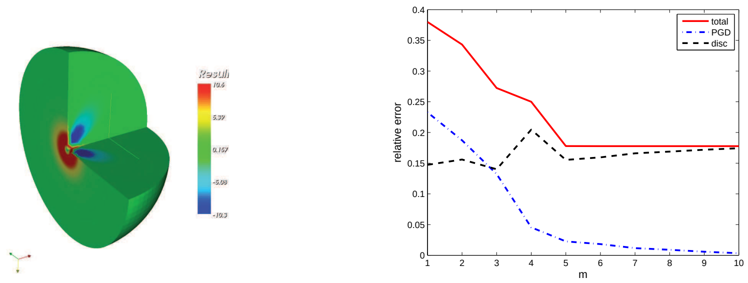

Figure 2. Example of 3D Green's function (left) and convergence of error sources with respect to PGD order m (right).

CONTROL OF MODELING ERRORS

The error estimation method based on the CRE can be extended to take into account modeling errors which are created in model reduction methods. A recent application has considered the case of computations performed using the Proper Generalized Decomposition (PGD) i.e. searching the solution of a multi-parameter mechanical problem as a finite sum of separated variables functions (or modes):

$$\mathbf{u}(x_1, x_2, \ldots, x_n) \approx \sum_{i=1}^{m} \phi_i(x_1)\psi_i(x_2)\ldots\xi_i(x_n) \tag{3}$$

where n (resp. m) is the number of parameters (resp. modes). In that framework, a consistent error estimate can be computed from a double approach (kinematic and static) that enables to get admissible fields. The estimate captures all error sources (space, time and other parameter discretizations, as well as truncation of the series in the PGD representation), and contributions of these sources can be identified in order to drive adaptive algorithms effectively (see Fig. 2).

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