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Verifying Calculations – Forty Years On

An Overview of Classical Verification Techniques for FEM Simulations

Springer

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ISSN 2191-530X ISSN 2191-5318 (electronic)
SpringerBriefs in Applied Sciences and Technology
ISBN 978-3-319-20552-6 ISBN 978-3-319-20553-3 (eBook)
DOI 10.1007/978-3-319-20553-3

Library of Congress Control Number: 2015943353

Springer Cham Heidelberg New York Dordrecht London

Printed on acid-free paper

Springer International Publishing AG Switzerland is part of Springer Science+Business Media (www.springer.com)

Preface

Numerical modeling and simulation is increasingly used as a complement to experimental modeling and analysis and as a design tool in engineering applications. Each of these numerical solutions is intrinsically carrying an error associated with the discretization (mesh) the modeler has decided to use. This decision is based on finding a tradeoff between the computational cost and the numerical quality. However, after almost forty years of worldwide and active research efforts, the problem of properly assessing and controlling the quality of the numerical simulations is still relevant and an issue of major interest. Currently, certain maturity has been reached and calculations for industrial applications can be verified and error bounds can be provided for many cases (even though they are rarely computed in practice). However, the design of sophisticated engineering systems requires increasingly complex and coupled modeling for which verification tools are missing. Furthermore, new issues are appearing as industry needs faster calculations for real-time decision making, design optimization, inverse analysis, or simulation-based control purposes, which urgently requires new strategies for mastering and certifying calculations, bounding errors, in particular in presence of uncertainties.

The present textbook is edited as a companion support of a pre-conference course given on the occasion of the ADMOS 2015 conference, held in Nantes (France) during June 7–10, 2015. It aims at providing the bases to error assessment tools, including state-of-the-art achievements on a posteriori verification in scientific computing. These topics pertain to the field of estimation of discretization errors associated with Finite Element simulations, with a focus on Computational Mechanics applications. This research discipline effectively enables to control the accuracy of numerical simulations and to drive adaptive algorithms. The document also aims at presenting recent advances and forthcoming research challenges on the subject. The content is made of four chapters written by expert researchers on the field, which present fundamental principles on

classical a posteriori verification methods: explicit residuals methods, implicit residual methods, smoothing (recovery) methods, and duality-based methods.

We expect this book will help the reader to acquire an overview and insights into classical and state-of-the art techniques and tools for numerical verification.

Ludovic Chamoin
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Explicit Residual Methods

Yvon Maday

Abstract Numerical methods are now well established for the approximation of the solution to partial differential equations. These simulations allow to better understand complex phenomenon and lead to their control and optimization. The accuracy of the solution needs nevertheless be certified and in some case improved and the measurement of the error between the exact solution to the problem and the approximated one provided by the computer simulation must be estimated. A large amount of research has been done in this direction. This paper summarizes some of the most classical approaches that are available and allow, at very little extra computational cost to certify the results. These are known as the explicit residual techniques.

Keywords A posteriori error estimation · Explicit residual techniques · Numerical convergence · Finite element method · Reduced basis approximation

1 Introduction

The numerical simulation of mathematical models, written under the form of a partial differential equation, performed on computers is most of the time centered on matrix inversion. Indeed, the numerical solution is sought in a finite dimensional space of functions provided with an appropriate basis set; the model is then transformed under the form of a system of possibly nonlinear equations involving the components of the numerical solution in the basis set. The choices of

- the finite dimensional space—denoted in what follows as X_N and is assumed to be of dimension $d(N)$
- the appropriate basis set of X_N

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L. Chamoin and P. Díez (eds.), *Verifying Calculations – Forty Years On*,
SpringerBriefs in Applied Sciences and Technology,
DOI 10.1007/978-3-319-20553-3_1

- the solution algorithms adequate for solving the linear and nonlinear equations associated with a suitable stopping criteria

determine at the end of the computation of a given problem the accuracy of the approximation. In addition, (i) on one hand, the mathematical analysis of the nature of the various models proposed in different fields has led to a classification of problems and a know how on the best way to approximate the solutions (elliptic, mixed, parabolic, hyperbolic problems, reaction, advection, diffusion dominant behavior, conservations laws…), (ii) on the other hand various discretization spaces, discretization approaches and algorithms have been proposed and the numerical analysis that has been performed on these various approximation methods has identified their properties and the requirements on the solution and the model that allow to get the full benefit from the discretization approaches. This allows, when one faces a new problem, to guide the construction of the numerical approximation and the understanding of what can be expected.

In addition to these a priori statements, when the approximated solution to a given model is computed, it is important to be able to measure the quality of what has been performed and also give indications on what should be done in order to improve the precision of the approximation. This is the aim of the a posteriori analysis. It allows to quantify, in some cases very accurately, the error between the exact solution to the given model and the approximated one, we refer to [1–3, 23] for more advanced monographs on the subject.

In opposition to what happens for approximation through interpolation for instance where at least some values of the exact solution are accessible explicitly, the definition of the solution through a model is only implicit, e.g. given under the abstract form: find u in a normed functional space—denoted in what follows as X—such that the functional equation $F(u) = 0$. In such a frame, the evaluation of the error between the (unknown) exact solution u and its approximation u_N in X_N, expressed like $u - u_N$, measured in some norm, is itself a problem. In the case where the problem is linear, the functional equation is written as $F(u) = Au - f$ where f is a given functional data and A is a linear operator. In order to be slightly more precise, we can assume that A is a continuous operator from X into a functional space Y, and f is assumed to be given in Y. In such a case, formerly at least, the solution u is given by $u = A^{-1} f$ hence

$$u - u_N = A^{-1} f - u_N = A^{-1}[f - Au_N] = -A^{-1} F(u_N) \tag{1}$$

hence a way to measure $u - u_N$ is to consider the expression $F(u_N) = Au_N - f$ that is defined to be the *residual* of the equation evaluated on the approximated solution u_N.

In what follows, we shall present some variations upon this subject dealing with the proper link between the error between u and u_N measured in some norm and the computation of the residual and its evaluation in some other norm. We refer to the chapter Residual type error estimators of A. Huerta and P. Diez where Implicit residual techniques are presented.

2 Fourier Approximation

Let us start with the simple setting of a problem provided with periodic boundary conditions, i.e. problems set over $\mathbb{R}^d$, $d = 1, 2$, or 3 where the functions we are considering are assumed to be 2π periodic in each direction. The problem can thus be restricted to a unit cell $\Omega = (0, 2\pi)^d$ of a periodic lattice $\mathscr{R}$ of $\mathbb{R}^d$.

The natural functional spaces in this frame are the periodic Lebesgue spaces $L^p_\sharp(\Omega)$ (resp. periodic Sobolev spaces $W^{m,p}_\sharp(\Omega)$, $m \in \mathbb{N}$), with $p \in \overline{\mathbb{R}}$, $1 \leq p \leq \infty$, defined as being the restriction to Ω of 2π-periodic functions in $L^p_{loc}(\mathbb{R}^d)$ (resp. of functions in $W^{m,p}_{loc}(\mathbb{R}^d)$) and we note $H^m_\sharp(\Omega)$ the spaces $W^{m,p}_\sharp(\Omega)$ when $p = 2$.

The natural discretization in this periodic settings consists in using a Fourier basis. We denote by $(X_N)_{N>0}$ the family of finite-dimensional subspaces of X defined by

$$X_N = \text{Span}\left\{e_{\boldsymbol{k}} : \boldsymbol{x} \mapsto e^{i\boldsymbol{k}.\boldsymbol{x}},\, |k_p| \leq N,\, p = 1, \ldots, d, \boldsymbol{k} = (k_1, \ldots, k_d) \in \mathbb{Z}^d\right\}.$$

Remind now that, for any $v \in L^2_\sharp(\Omega)$,

$$v(\boldsymbol{x}) = \sum_{\boldsymbol{k}\in\mathbb{Z}} \widehat{v}_{\boldsymbol{k}} e_{\boldsymbol{k}}(\boldsymbol{x}),$$

where $\widehat{v}_{\boldsymbol{k}}$ is the $\boldsymbol{k}$th Fourier coefficient of v:

$$\widehat{v}_{\boldsymbol{k}} := \int_\Omega v(\boldsymbol{x})\, \overline{e_{\boldsymbol{k}}(\boldsymbol{x})}\, d\boldsymbol{x} = \int_\Omega v(\boldsymbol{x})\, e^{-i\boldsymbol{k}.\boldsymbol{x}}\, d\boldsymbol{x}.$$

For any integer m, we now endow the Sobolev space $H^m_\#(\Omega)$ with the equivalent norm expressed in Fourier modes as follows

$$\|v\|_{H^m} = \left(\sum_{\boldsymbol{k}\in\mathbb{Z}^d} \left(1 + |\boldsymbol{k}|^2\right)^m |\widehat{v}_{\boldsymbol{k}}|^2\right)^{1/2}, \tag{2}$$

and we note that the definition of this scale of spaces can be actually extended over real indices s (the spaces $H^s_\#(\Omega)$ associated with negative values of s correspond to the dual spaces of $H^{-s}_\#(\Omega)$). In what follows we shall use only this definition of the H^s–norm (2). We obtain that for any $r \in \mathbb{R}$, and all $v \in H^r_\#(\Omega)$, the best approximation of v in $H^s_\#(\Omega)$ for any $s \leq r$ is

$$\Pi_N v = \sum_{\boldsymbol{k}\in\mathbb{Z}, |\boldsymbol{k}|\leq N} \widehat{v}_{\boldsymbol{k}} e_{\boldsymbol{k}}. \tag{3}$$

The more regular v (the regularity being measured in terms of the Sobolev norms H^r), the faster the convergence of this truncated series to v: for any real numbers r and s with $s \leq r$, we have, see e.g. [8]