Interval Finite Element Methods: New Directions

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1. Introduction

Many problems in computational engineering and science, such as solid and fluid mechanics, electromagnetics, heat transfer, or chemistry, are sufficiently well described on the macroscopic level in terms of partial differential equations (PDEs). In practice, these processes may be very complex, and the presence of multiple spatial and/or temporal scales, or even discontinuities in the solution, often makes their computer simulation challenging. There exist advanced numerical methods to tackle these problems, such as finite element methods (FEM). Lately, new advanced version of these methods have appeared, such as hierarchic higher-order finite element methods (*hp*-FEM) and extended finite element methods (X-FEM). Most of these methods work on a traditional basis where no uncertainty considerations are present in the modeling or computation. However, the need for numerical treatment of uncertainty becomes increasingly urgent. In many cases a given problem can be solved efficiently and accurately for a given set of input data (such as geometry, boundary conditions, material parameters, etc.), but little can be said about how the solution depends on uncertainties in these parameters.

However, the design of an engineered system requires the performance of the system to be guaranteed over its lifetime. One of the major difficulties a designer must face is that neither the external demands of the systems nor its manufacturing variations are known exactly. In order to overcome this uncertainty, the designer must provide excessive capabilities and over design the system. As analysis tools continue to be developed, the predictive skills of designers have become finer. In addition, the demands of the market place require that more efficient designs be developed. In order to satisfy these current requirements in designs subject to uncertainties, the uncertainties in the performance of the system must be included in the analysis.

At present, analytical and Monte-Carlo techniques are used to handle probabilistic uncertainty, and interval finite element methods are used to handle interval uncertainty. In many practical situations, we have both probabilistic and interval uncertainty. The problem of efficient combination of probabilistic and interval uncertainties have to be explored for problems where neither Monte Carlo nor standard interval methods can be used. Therefore, advanced interval arithmetic techniques, ideally handling probabilistic uncertainty as well, need to be implemented into modern finite element methods both on the practical and theoretical levels. When developing these techniques, we need to take into account recent developments in interval computation techniques are their applications and developments in promising finite element techniques such as *hp*-FEM and X-FEM, together with results obtained with interval finite element methods for problems of structural mechanics (reviewed in Section 2).

2. Interval Finite Element Methods: A Brief Overview

There are various ways in which the types of uncertainty might be classified. One is to distinguish between "aleatory" (or stochastic) uncertainty and "epistemic" uncertainty. The first refers to underlying, intrinsic variabilities of physical quantities, and the latter refers to uncertainty which might be reduced with additional data or information, or better modeling and better parameter estimation (Melchers, 1999). Probability theory is the traditional approach to handle uncertainty. This approach requires sufficient statistical data to justify the assumed statistical distributions. Analysts agree that, given sufficient statistical data, the probability theory describes the stochastic uncertainty well. However, traditional probabilistic modeling techniques cannot handle situations with incomplete or little information on which to evaluate a probability, or when that information is nonspecific, ambiguous, or conflicting (Walley, 1991; Ferson and Ginzburg, 1996; Sentz and Ferson, 2002). Many generalized models of uncertainty have been developed to treat such situations, including fuzzy sets and possibility theory (Zadeh, 1978), Dempster-Shafer theory of evidence (Dempster, 1967; Shafer, 1976), random sets (Kendall, 1974), probability bounds (Berleant, 1993; Ferson and Ginzburg, 1996; Ferson et al., 2003), imprecise probabilities (Walley, 1991), convex models (Ben-Haim and Elishakoff, 1990), and others.

These generalized models of uncertainty have a variety of mathematical descriptions. However, they are all closely connected with interval analysis (Moore, 1966), in which imprecision is described by an interval (or, more generally, a set). For example, a fuzzy number can be viewed as a nested collection of intervals corresponding to different levels of confidence α (so-called α-cuts). Thus, the mathematical analysis associated with fuzzy set theory can be performed as interval analysis on different α-levels (Muhanna and Mullen, 1995; Lodwick and Jamison, 2002), and fuzzy arithmetic can be performed as interval arithmetic on α cuts. A Dempster-Shafer structure (Dempster, 1967; Shafer, 1976) with interval focal elements can be viewed as a set of intervals with probability mass assignments, where the computation is carried out using the interval focal sets. Probability bounds analysis (Berleant, 1993; Ferson and Ginzburg, 1996; Ferson et al., 2003) is a combination of standard interval analysis and probability theory. Uncertain variables are decomposed into a list of pairs of the form (interval, probability). In this sense, interval arithmetic serves as the calculation tool for the generalized models of uncertainty.

Recently, various generalized models of uncertainty have been applied within the context of the finite element method to solve a partial differential equation with uncertain parameters. Regardless what model is adopted, the proper interval solution will represent the first requirement for any further rigorous formulation. Finite element method with interval valued parameters results in Interval Finite Element Method (IFEM). The numerical solution of an IFEM is the focus of this section. Different formulations of IFEM have been developed. The use of IFEM solution techniques can be broadly classified into two groups, namely the optimization approach and the non-optimization approach.

In the optimization approaches (Koyluoglu et al., 1995; Rao and Chen, 1998; Akpan et al., 2001; Möller et al., 2000), optimizations are performed to compute the minimal and maximal structural responses when the uncertain parameters are constrained to belong to intervals. This approach often encounters practical difficulties. Firstly it requires efficient and robust optimization algorithm. In most structural engineering problems, the objective function is nonlinear and complicated, thus often only an approximate solution is achievable. Secondly, this approach is computationally expensive. For each response quantity, two optimization problems must be solved to find the lower and the upper bounds.

More recently, non-optimization approaches for the interval finite element analysis have been developed in a number of papers. For linear elastic problems, this approach leads to a system of linear interval equations, then the solution is sought using various methods developed for this purpose. The major difficulty associated with this approach is the "dependency problem" (Moore, 1979; Neumaier, 1990; Hansen, 1992; Muhanna and Mullen, 2001). In general, dependency problem arises when one or several interval variables occur more than once in an interval expression. The dependency in interval arithmetic leads to an overestimation of the solution. A straightforward replacement of the system parameters with interval ones without taking care of the dependency problem is known as a naïve application of interval arithmetic in finite element method (naïve IFEM). Usually such a use results in meaninglessly wide and even catastrophic results (Muhanna and Mullen, 2001).

In the non-optimization category, a number of developments can be presented. A combinatorial approach (based on an exhaustive combination of the extreme values of the interval parameters) was used in (Muhanna and Mullen, 1995; Rao and Berke, 1997). This approach gives exact solution in special cases of linear elastic problems. However, it is computationally tedious and expensive, and is limited to the solutions of small-scale problems.

A convex modeling and superposition approach was proposed to analyze load uncertainty in (Pantelides and Ganzerli, 2001), and exact solution was obtained. However, the superposition is only applicable to load uncertainty.

A combinatorial approach was used in (Ganzerli and Pantelides, 1999) to treat interval modulus of elasticity.

A static displacement bounds analysis was developed in (Chen et al., 2002) have developed using matrix perturbation theory. The first-order perturbation was used and the second-order term was neglected. The result is approximate and not guaranteed to contain the exact bounds.

The paper (McWilliam, 2000) proposed two methods for determining the static displacement bounds of structures with interval parameters. The first method is a modified version of perturbation analysis. The second method is based on the assumption that the displacement surface is monotonic. However, for the general case, the validity of monotonicity is difficult to verify.

In (Dessombz et al., 2001), an interval FEM was introduced in which the interval parameters were factored out during the assembly process of the stiffness matrix. Then an enhanced iterative algorithm from (Rump, 1983) was employed for solving the linear interval equation. In this work, the overestimation control becomes more difficult with the increase of the number of the interval parameters, which does not lead to useful results for practical problems.

In (Muhanna and Mullen, 1995; Mullen and Muhanna, 1996; Mullen and Muhanna, 1999), an interval-based fuzzy finite element has been developed for treating uncertain loads in static structural problems. Load dependency was eliminated, and the exact solution was obtained. Also, in (Muhanna and Mullen, 2001), an interval FEM was developed based on an element-by-element technique and Lagrange multiplier method. Uncertain modulus of elasticity was considered. Most sources of overestimation were eliminated, and a sharp result for displacement was obtained. However, this formulation can only handle uncertain modulus of elasticity, and it can not obtain the sharp enclosures for element internal forces.

A new formulation for interval finite element analysis for linear static structural problems is developed in the work of (Muhanna et al., 2005). Material and load uncertainties are handled simultaneously, and sharp enclosures on the system's displacement as well as the internal forces are obtained efficiently.

Recently, new advancements has been made in the area of interval FEM, e.g., (Corliss et al., 2004; Popova et al., 2003), and the significant development in (Neumaier and Pownuk, to appear) where sharp results are achieved for linear truss problems even with large uncertainty.

3. First Challenge: Combination of Interval and Probabilistic Techniques

In many problems, e.g., of fundamental physics, one knows the exact equations, one knows the exact values of the parameters of these equations, and all one needs is to solve these equations as fast and as accurately as possible. These are the cases when the traditional FEM techniques directly lead to practically useful results. In engineering practice one approximates both the actual computational domain and function space using a collection of finite elements, the FEM solution only is an approximation to the actual continuous field, but as one increases the number and/or polynomial degree of the finite elements (using h, p, or hp-adaptivity), the FEM results become more and more accurate, and at some point one gets the desired solution with a very high accuracy.

There are many other application problems, however, where one only knows the approximate equations, or where one knows the equations, but one only knows the approximate values of the corresponding parameters. For example, in many civil engineering problems, one does not know the exact values of the Young modulus; one only knows the bounds for these values coming from the fact that one knows the material, and one knows the bounds for this type of material. In such problems, even if one uses an extremely fine mesh to make the discretization error negligible, the resulting FEM solution may still be very different from the actual behavior of an analyzed system – because of the uncertainty in the parameters and/or equations.

In such situations, to make the FEM results practically useful, one must be able to estimate how different the true and approximate solutions can be. In other words, one needs to be able to estimate how the uncertainty in the parameters of the system can affect the FEM results.

This question is of paramount importance in science and engineering, and, of course, there has already been a lot of research aiming to answer this question. Most of this research is based on the assumption that one knows the exact probability distributions corresponding to all uncertain parameters. In this stochastic FEM case one can, in principle, apply the Monte Carlo method: Simulate all the parameters according to their known distributions, apply FEM for the system with the simulated values of the corresponding parameters, and then perform the statistical analysis of the FEM results – and thus, get the probability distribution for these results.

This stochastic FEM approach works well in many practical situations. In many other situations, on the other hand, the probabilities of different values of the uncertain parameters are not known. For example, in civil engineering one often only knows the lower and upper bounds on the Young modulus, but the probabilities of different values within the corresponding interval may depend on the manufacturing process, and thus they may differ from one building to another dramatically. In situations which require reliable estimates, e.g., when one analyzes the stability of a building, it is not enough to select one possible distribution and confirm that the building is stable under this distribution; to get a reliable result, one must make sure that the building remains stable for all possible distributions on the given interval.

Lately, there has been a lot of progress in applying interval computation techniques to FEM with interval uncertainty. This area of research was started in the early 1990s, and it was advanced in the series of papers reviewed in Section 3.

The software tools developed recently by R. Muhanna in the U.S., as well as similar tools developed by A. Neumaier in Austria, allowed us to prove reasonable interval FEM estimates – at least for the situations like civil engineering, when one can get a reasonable description of a structure by using several hundreds of finite elements only. These methods have led to very useful practical applications to the reliability of buildings and associated problems.

However, there still are practical problems for which the interval FEM is not fully adequate. As of now, there are two main methods to handle uncertainty in FEM problems:

- Stochastic FEM methods for situations when one knows the exact probability distribution of all uncertain parameters.
- Interval FEM methods for situations when no information about the probability distributions is available – one only knows the intervals of possible value of these parameters.

In other words, at present one only knows how to handle uncertainty in two extreme situations:

- One has full information about the probabilities.
- One has no information about the probabilities.

Many practical situations lie in between these two extremes: one has a partial information about the probabilities. For example, one may also have interval bounds for some of the parameters, but one may know the probability distribution for other parameters. For example, one may know only intervals of possible values of the manufacturing-related parameters, but, when one has good records, one may also know probabilities of different values of, say, weather-related parameters.

It is therefore highly desirable to extend the interval and stochastic FEM techniques to the case when one has a combination of interval and probabilistic uncertainty. Extension of interval and statistical methods to such a technique is, at present, an active area of research. While these combined techniques have been developed and applied to different practical situations, there are still very few applications to FEM.

Our preliminary results have already led to an idea of such an extension for an important case when one has interval uncertainty for some parameters and probabilistic uncertainty for some other parameters. In such situations, one can apply Monte Carlo techniques to simulate parameters with known probability distributions. For each such simulation, one can then use interval FEM techniques to take into account the corresponding interval uncertainty. As a result of applying interval FEM techniques, one gets the interval bounds for the resulting FEM inaccuracy. By repeating this simulation several times, one gets several bounds – and hence, the resulting bounds distribution. By using this bounds distribution, one can now supplement the interval FEM information that the FEM inaccuracy Δy is bounded by a certain value Δ with the information that with probability 90%, one can get a narrower bound that bounds Δy in at least 90% of the case, yet narrower bound which holds in at least 80% of the cases, etc. Similar techniques need to be developed and applied to more complex situations with combined interval and probabilistic uncertainty.

Comment. The above idea is applicable in situations in which we already have well-developed interval FEM techniques. Another important research topic is the extension of interval FEM techniques to other advanced FEM techniques such as *hp*-FEM. These adaptive higher-order FEM techniques has proved to be superior to traditional lowest-order FEM in many practical problems, both in terms of higher accuracy and dramatically smaller size of the resulting stiffness matrices and substantially shorter CPU time; see, e.g., see (Demkowicz et al., 2001; Šolín, 2005) and the references therein.

4. Second Challenge: Nonlinear FEM with Stochastic Variations and Uncertainty for Microstructure

Significant amount of work was done in the use of both the probabilistic and non-probabilistic finite element methods for the assessment of uncertainty for linear PDEs. Several methods have proven to be successful: stochastic methods, interval methods, fuzzy number methods (Elishakoff and Ren, 1999; Haldar and Mahadevan, 2000; Schuëller, 2001). These approaches have been primarily applied to problems academic in nature. The issue of uncertainty and verification in practical engineering problems still seems to be a little addressed issue. By verification one is referring to the definition from (Babuška and Oden, 2004), where correct empirically derived model parameters are used.

An area of emerging importance is the application of stochastic and interval finite element methods to nonlinear continuum mechanics problems. Specifically, effects of uncertainty in the microstructural state of materials need to be studied. In this area, enriched finite element methods, particularly the extended finite element methods (X-FEM) (Moës et al., 1999; Belytschko et al., 2001; Stazi et al., 2003), need to be combined with interval and stochastic methods to investigate the effect of uncertainty on the position and state of the microstructure.

The X-FEM uses a local partition of unity technique to construct finite elements which are capable of reproducing discontinuities and singularities without mesh refinement. This approach has been used to model crack growth (Moës et al., 1999; Chen and Belytschko, 2003; Stazi et al., 2003), material inhomogeneities (Sukumar et al., 2000; Chessa et al., 2003) as well as various other phenomena (Chessa et al., 2002; Chessa and Belytschko, 2003; Chessa and Belytschko, to appear). In all of these methods, the location of the material interfaces is implicitly defined by a level set field (Sethian, 1999). Thus, material models with a significantly increased number of defects and inclusions are computationally tractable.

This technique should be extended to non-linear problems of fracture mechanics, e.g., to non-linear Stefan-type equations that describe the dynamics of crack growth.

In principle, both for linear and nonlinear problems, we can use a straightforward perturbation approach as in (Liu et al., 1999). However, such approaches allow for only small variations in the variables. To allow for large stochastic variations, a combined approach of interval finite element methods and homogeneous chaos methods need to be developed.

5. Third Challenge: Enhancing *hp*-FEM with Advanced Interval Techniques

The *hp*-FEM is distinguished from the traditional FEM by combining elements of variable size and polynomial degree to achieve extremely fast convergence. The method originates in the early works of I. Babuška et al. (Babuška and Gui, 1986; Babuška et al., 1999). In the last few years, significant progress was made towards the solution of practical problems related to the computer implementation of the *hp*-FEM (design of optimal algorithms and data structures, automatic *hp*-adaptive strategies, optimal higher-order shape functions, etc.), see (Ainsworth and Senior, 1997; Karniadakis and Sherwin, 1999; Paszynski et al., 2004; Rachowicz et al., 2004; Šolín et al., 2003; Šolín and Demkowicz, 2004). Typically, the *hp*-FEM is capable of solving PDE problems using dramatically fewer degrees of freedom compared to standard FEM. Several such examples, obtained using a modular *hp*-FEM system HERMES which is being developed at the University of Texas at El Paso, are presented in the recent monograph (Šolín, 2005). It is therefore desirable to extend interval FEM techniques to *hp*-FEM.

We believe that for *hp*-FEM, the existing interval techniques will be even more efficient than for more traditional FEM techniques. Indeed, one of the main advantages of *hp*-FEM in comparison to lowest-order methods is that in many practical situations, for the same approximation accuracy, *hp*-FEM techniques require dramatically fewer degrees of freedom (unknown solution coefficients). In other words, they can decrease the size of the matrices in the corresponding linear systems substantially. When we solve systems of linear equations with interval uncertainty, in general, we get enclosures with excess width, and this excess width drastically increases with the size of a system. Thus, the decrease in the system's size will allow us to get more accurate estimates for the resulting interval uncertainty.

6. Fourth Challenge: Using Interval Computations to Prove Results about FEM Techniques

Finally, it is desirable to use interval computation techniques – techniques which provide guaranteed bounds for functions on continuous domains – in proving results about FEM methods, results which should be valid for all possible values of the corresponding parameters. In this section, we describe our preliminary results in this direction and related challenges.

6.1. Formulation of the Problem

Our preliminary results are related to elliptic partial differential equations $Lu = f$. The simplest case to begin with is the one-dimensional Poisson equation $-u'' = f$ with homogeneous Dirichlet boundary conditions.

For elliptic differential equations $Lu = f$, there is a known *Maximum Principle*: If $f(x) \leq 0$ for all points x from the domain Ω, then (under reasonable smoothness conditions) the solution u attains its maximum on the boundary of Ω. Because of the maximum principle:

- for the same f, we have a continuous dependence of the solution on the boundary conditions: namely, if u_1 and u_2 are two solutions with the same right-hand side f, then the sup-norm distance $\sup\limits_{x\in\Omega} |u_1(x) - u_2(x)|$ between u_1 and u_2 (defined as the supremum over *all* x from Ω) is equal to the supremum $\sup\limits_{x\in\partial\Omega} |u_1(x) - u_2(x)|$ of the difference over the boundary $\partial\Omega$ of the domain Ω;
- similarly, there is a continuous dependence of u on f.

This allows us to provide *guaranteed bounds* on the solution based on the uncertainty with which we know the right-hand side f and the boundary values of u.

In the Finite Element Method we consider piecewise-polynomial functions $u_{h,p}(x)$ (which span a finite-dimensional space $V_{h,p}$. Of course, $u_{h,p}$ is not an exact solution of the original problem $Lu = f$. Instead, we look for an exact solution to the *discrete weak formulation* of the partial differential equation, see, e.g., (Šolín, 2005).

It is known that, sometimes, $f(x) \leq 0$ for all $x \in \Omega$, but the maximum of the resulting finite element solution $u_{h,p}$ is not necessarily attained on the boundary. As a result,

- even when we know the bounds on the uncertainty in f and in the boundary conditions, it is difficult to find guaranteed bounds on the uncertainty in $u_{h,p}$,
- the approximate solution $u_{h,p}$ may be unphysical, e.g., it may attain negative values when it represents absolute temperature, concentration, etc.

It is therefore desirable to find discrete analogues of the classical maximum principles, which are called *discrete maximum principles*. Such analogues are known for lowest-order (piecewise linear) FEM since the early 1970s (Ciarlet, 1970; Ciarlet et al., 1973). For the latest results, see, e.g., (Korotov et al., 2000; Křížek and Liu, 2003; Karátson and Korotov, 2005).

Until recently, no extensions to higher-order FEM were known. Moreover, a rather discouraging result (Höhn and Mittelmann, 1981) stated that the discrete maximum principle did not hold for the Poisson equation $-u'' = f$ discretized with quadratic elements except with unrealistic conditions on the triangulation. After that, it was assumed for a long time that no discrete maximum principles for *hp*-FEM can be proved.

In (Šolín and Vejchodský, 2005), we solved the Poisson equation in one spatial dimension, equipped with homogeneous Dirichlet boundary conditions $u(-1) = u(1) = 0$ and with a right-hand side $f(x) = 200 \cdot \mathrm{e}^{-10\cdot(x+1)}$. According to the standard maximum principle, the actual solution $u(x)$ is nonnegative in the entire interval $(-1, 1)$. Let us consider this whole domain as a single element, and let us approximate the desired solution by a 3-rd degree polynomial $u_{h,p}(x)$ which satisfies the desired boundary conditions $u_{h,p}(-1) = u_{h,p}(1) = 0$. We want $-\int_{-1}^{1} u'_{h,p}(x)v'(x) - f(x)v(x)\,\mathrm{d}x = 0$ for all 3-rd other polynomials $v(x)$ such that $v(\pm 1) = 0$.

Due to linearity of the problem, the satisfaction of this integral condition for *all* these polynomials is equivalent to the fact that this condition must hold for any basis, for example, $v_1(x) = 1 - x^2$, $v_2(x) = x(1 - x^2)$. Thus, in terms of the coefficients of the unknown polynomial $u_{h,p}(x)$, we get an easy-to-solve system of linear equations, whose solution

$$u_{h,p}(x) = \frac{1}{40} \cdot \left[54 + 66 \cdot \mathrm{e}^{-20} - (73 - 133 \cdot \mathrm{e}^{-20}) \cdot x\right] \cdot \left(1 - x^2\right)$$

is negative, e.g., at $x = 0.9$.

6.2. Formulation of the Result

The reason for the above negativity is that, as one can easily check, the weak solution corresponding to the original function $f(x)$ is the same as the weak solution corresponding to the *projection* $f_{h,p}(x)$ of the function $f(x)$ on the set of polynomials of 3-rd degree – i.e., for the 3-rd degree polynomial $f_{h,p}(x)$ for which $\int (f(x) - f_{h,p}(x)) \cdot v(x)\,\mathrm{d}x = 0$ for all 3-rd degree polynomials $v(x)$. For the above function $f(x)$, the projection

$$f_{h,p}(x) = -8.25 + 29.175 \cdot x + 54.75 \cdot x^2 - 93.625 \cdot x^3$$

is no longer nonnegative: e.g., it is negative for $x = 0$.

It is therefore reasonable to ask whether the Discrete Maximum Principle for higher-order FEM holds if we restrict ourselves to the case when not only the function $f(x)$ is nonnegative, but its projection $f_{h,p}(x)$ (i.e., the polynomial of the corresponding degree) is nonnegative as well.

So, we arrive at the following problem. For some integer p, we have a p-th degree polynomial $f_{h,p}(x)$ defined on the interval $(-1, 1)$. We are looking for a weak solution $u_{h,p}(x)$ to the equation $-u'' = f$ with the boundary conditions $u(-1) = u(1) = 0$, i.e., for a polynomial $u_{p,h}(x)$ of p-th degree for which $\int_{-1}^{1}(-u''_{h,p}(x) - f(x)) \cdot v(x)\,\mathrm{d}x = 0$ for all polynomials $v(x)$ of degree p. We want to prove that if the polynomial $f_{h,p}(x)$ is nonnegative on the entire interval $(-1, 1)$, then the weak solution $u_{h,p}(x)$ is also nonnegative for all $x \in (-1, 1)$. By using interval computations, we can prove this statement for $p = 2, 3, 4, \ldots, 10$; see (Šolín and Vejchodský, 2005; Šolín, 2005) for details.

6.3. How We Use Interval Computations

To prove the above result, we use a special basis in the linear space of all polynomials of p-th degree which vanish for $x = -1$ and $x = 1$: the basis of *Lobatto shape functions* (see, e.g., (Šolín, 2005))

$$l_k(x) = \frac{1}{\|L_{k-1}\|_{L^2}} \cdot \int_{-1}^{x} L_{k-1}(\xi)\,\mathrm{d}\xi, \quad 2 \le k,$$

where $L_0, L_1, \ldots$ are Legendre polynomials with $\|L_{k-1}\|_{L^2} = \sqrt{2/(2k-1)}$. In terms of these functions, the general solution to the above problem can be represented in the following form

$$u_{h,p}(x) = \int_{-1}^{1} f_{h,p}(z) \cdot \Phi_p(x,z)\,\mathrm{d}z, \tag{1}$$

where the *Green's function* $\Phi_p(x,z)$ has the form

$$\Phi_p(x,z) = \sum_{i=1}^{p-1} l_{i+1}(x) \cdot l_{i+1}(z).$$

For every $p > 1$, the function $\Phi_p(x,z)$ is a given bivariate polynomial defined in the square $(-1,1)^2$. We want to use the expression (1) to prove that $u_{h,p}(x)$ is nonnegative for all $x \in (-1,1)$. This is done in two steps:

1. First, we identify a subdomain Ω_p^+ of the interval $(-1,1)$ where the function Φ_p is positive.
2. After that, we find a quadrature rule of the order of accuracy $2p$ (exact for all polynomials of degree less or equal to $2p$) with positive weights and points lying in Ω_p^+.

The construction of the subdomains Ω_p^+ and the corresponding quadrature rules finishes the proof. The concrete subdomains Ω_p^+ along with the quadrature rules can be found in (Šolín and Vejchodský, 2005).

The interval computation technique is used to verify that the functions Φ_p are positive in the subdomains Ω_p^+. Let us demonstrate the procedure on the quartic case, where we deal with the function $\Phi_4(x,z) = \sum\limits_{i=1}^{3} l_{i+1}(x) \cdot l_{i+1}(z)$. Since each polynomial $l_i(x)$ vanishes at $x = -1$ and at $x = 1$, this polynomial is proportional to $(x+1)\cdot(x-1) = x^2 - 1$, so the Green's function $\Phi_4(x,z)$ can be represented as $\Phi_4(x,z) = (x^2-1)\cdot(z^2-1)\cdot\Psi_4(x,z)$, where

$$\Psi_4(x,z) = \frac{3}{8} + \frac{5}{8} \cdot x \cdot z + \frac{7}{128} \cdot (5x^2 - 1) \cdot (5z^2 - 1). \tag{2}$$

The graph of the function $\Phi_4(x,z)$ is shown in Fig. 1.

To prove that the Green's function $\Phi_4(x,z) = (x^2-1)\cdot(z^2-1)\cdot\Psi_4(x,z)$ is nonnegative in the entire square $[-1,1]^2$, it is sufficient to prove that $\Psi(x,z) \geq 0$ for all $(x,z) \in [-1,1]^2$. We prove this nonengativity by using straightforward interval computations; see, e.g., (Jaulin et al., 2001).

In interval computations, one deals with intervals instead of numbers, and standard unary and binary operations are extended from numbers to intervals in a natural way. For example, $[\underline{a}, \overline{a}] + [\underline{b}, \overline{b}] = [\underline{a} + \underline{b}, \overline{a} + \overline{b}]$, $[\underline{a}, \overline{a}] - [\underline{b}, \overline{b}] = [\underline{a} - \overline{b}, \overline{a} - \underline{b}]$, and so on. If we replace every operation with numbers by the corresponding operation of interval arithmetic, we get an enclosure for the range of the analyzed function on given intervals (Jaulin et al., 2001).

Let us use this technique to prove the nonnegativity of the function $\Psi_4(x,z)$ in the square $[-1,1]^2$: Substituting a pair of intervals $X = [\underline{x}, \overline{x}]$ and $Z = [\underline{z}, \overline{z}]$ into the formula for $\Psi_4(x,z)$, we obtain an enclosure

$$[\underline{\Psi}_4, \overline{\Psi}_4] \supseteq \Psi_4(X,Z) = \{\Psi_4(x,z);\; x \in X, z \in Z\}.$$

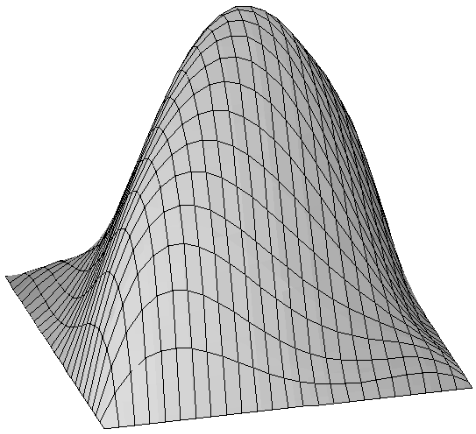

Figure 1. The function $\Phi_4(x, z)$.

Since the function $\Psi_4(x, z)$ is polynomial and it only contains rational coefficients, its evaluation for rational intervals can be done using exact integer arithmetic.

Step 1: Consider the intervals $X_1 = Z_1 = [-1, 1]$, and compute the enclosure $[\underline{\Psi}_4, \overline{\Psi}_4]$ for $\Psi_4(X_1, Z_1)$:

$$[\underline{\Psi}_4, \overline{\Psi}_4] = [-25/16, 95/32] \supseteq \Psi_4(X_1, Z_1).$$

If the left endpoint $\underline{\Psi}_4$ of the enclosure interval $[\underline{\Psi}_4, \overline{\Psi}_4]$ was nonnegative, then the proof would be finished. Since this is not the case, we refine the grid by halving both the intervals X_1 and Z_1. We obtain four subdomains $[-1, 0] \times [-1, 0]$, $[-1, 0] \times [0, 1]$, $[0, 1] \times [-1, 0]$, and $[0, 1] \times [0, 1]$.

Step 2: Compute the enclosures for these subdomains:

– for $[-1, 0] \times [-1, 0]$, we get $[\underline{\Psi}_4, \overline{\Psi}_4] = [5/32, 15/8] \supseteq \Psi_4([-1, 0], [-1, 0])$;

– for $[-1, 0] \times [0, 1]$, we get $[\underline{\Psi}_4, \overline{\Psi}_4] = [-15/32, 5/4] \supseteq \Psi_4([-1, 0], [0, 1])$;

– for $[0, 1] \times [-1, 0]$, we get $[\underline{\Psi}_4, \overline{\Psi}_4] = [-15/32, 5/4] \supseteq \Psi_4([0, 1], [-1, 0])$;

– for $[0, 1] \times [0, 1]$, we get $[\underline{\Psi}_4, \overline{\Psi}_4] = [5/32, 15/8] \supseteq \Psi_4([0, 1], [0, 1])$.

This proves that the function Ψ_4 (and hence also Φ_4) is nonnegative in the subdomains $[-1, 0] \times [-1, 0]$ and $[0, 1] \times [0, 1]$. As for the remaining subdomains $[-1, 0] \times [0, 1]$ and $[0, 1] \times [-1, 0]$, we divide each of them into four equal subdomains, compute the enclosure for each new subdomain, etc.

After five iterations of this procedure, we get a partition of $[-1, 1]^2$ for which the left endpoints of the enclosures are nonnegative. So we have proved that Ψ_4 (and hence also Φ_4) is nonnegative in $[-1, 1]^2$.

The Java programs and output files with details on the computations for $p = 4, 5, \ldots, 10$ can be viewed on the web page http://www.math.utep.edu/Faculty/solin/intcomp

6.4. New Challenges

Can we extend the above one-dimensional result to a multi-dimensional case? The following example shows that the assumption of nonnegativity of the polynomial L^2-projection of the right-hand side f will no longer be sufficient.

To illustrate this, let us consider a triangular domain Ω given by the vertices $[-1, -1]$, $[1, -1]$, $[-1, 1]$, and the stationary heat transfer equation $-\Delta\theta = f$ in Ω equipped with zero Dirichlet boundary conditions $\theta(\boldsymbol{x}) = 0$ for all $\boldsymbol{x} \in \partial\Omega$. The heat sources f are chosen to be a nonnegative cubic polynomial $f(x_1, x_2) = 1000 \cdot (x_1 + 1)^3$. In this case the exact solution θ is nonnegative in the domain Ω due to the classical (continuous) maximum principle for the Poisson equation.

The problem is discretized using a one-element mesh $K = \Omega$ with the polynomial degree $p(K) = 10$. It is shown in Fig. 2 that the approximate temperature $\theta_{h,p}$ is negative, i.e., nonphysical, near the right corner of Ω.

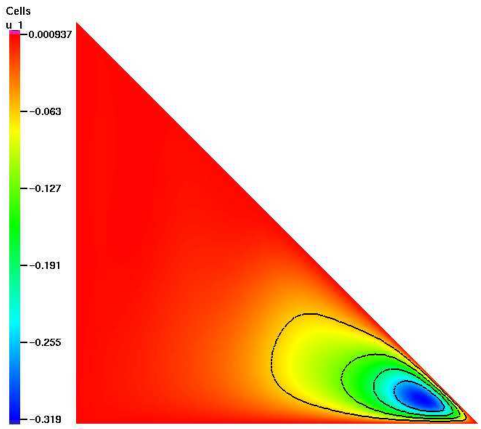

Figure 2. Nonphysical finite element solution of stationary heat transfer equation with zero boundary conditions and positive heat sources.

The formulation of conditions on the data and/or triangulation, which would guarantee the nonnegativity of the approximate solution, are an open problem. So far, we have found only partial conditions. Once these conditions are found, we will need to sue interval computation techniques to prove the desired nonnegativity.

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