Review of the Doctoral Thesis

A posteriori error estimates for numerical solution of convection-diffusion problems

by

Ivana Šebestová.

Reviewer: Assoc. Prof. Dr. Jan H. Brandts, University of Amsterdam, Netherlands.

This review will consist of an outline of the thesis followed by comments on original contributions of the applicant as can be found in her thesis. Then I will give my opinion on the mathematical content of the thesis, including some criticism. I end with my recommendation.

1. Outline

The thesis starts with an introduction (pp.7–10) for non-specialists followed by an introductory chapter (pp.11-18) in which the Laplace equation and the heat equation are introduced together with their respective discretizations by *interior penalty Discrete Galerkin* methods.

In Chapter 2 (pp.19–36), *a posteriori* error estimates are developed for the *spatial* discretization of the heat equation in comparison to the *semi-discretization* by the *implicit Euler* method, using *discrete Helmholz decompositions.* A numerical experiment is performed.

In Chapter 3 (pp.37–75), an existing *a posteriori* error estimator for the Laplace equation, explained in Section 1.2.4, is generalized such that hanging nodes and variable polynomial degree of approximation are allowed, and also the *algebraic error* is included in the analysis. The developed estimator is tested numerically, resulting in twenty pages (pp.56–75) of data, represented in the form of graphs and error distribution plots.

The final chapter, Chapter 4 (pp.76–94) is about an altogether different topic, which is the estimation of constants that appear in various, often-used, inequalities, such as the *Poincaré-Friedrichs inequality* and the *trace-inequality.* It is claimed (in the introduction) that, contrary to what can be found in the existing literature, *guaranteed lower bounds* for such constants are developed.

2. Quality and originality of the results

Chapters 2,3, and 4 contain original research results of the applicant and her co-authors. Some of the results are generalizations and adaptations of existing results and techniques, whereas others, particularly in Chapter 4, are of a more creative and innovative nature. The results of the first mentioned type are highly technical and useful in their own context: Section 2.2 and 2.3 contain the main theorems on error estimation for the heat equation. Both are complicated and technical results relying on several lemmas that were developed in Section 2.1. Similarly, in Section 3.2-3.4, the error estimators for the Laplace equation are rather involved and tedious and working out the details requires good insight in several aspects of applied mathematics. For both chapters it holds that implementing the methods and their error estimators into an adaptive finite element code is a nontrivial task that proves that the applicant has deep knowledge of the methods she studied, as well as excellent programming skills. The main ideas of Chapter 4 are much less technical, and both more generally, and more widely applicable. They are in a mathematical sense simpler (meaning: less technical), and convey several interesting ideas in functional analysis. Moreover, the problem of finding lower bounds for the smallest singular value of a linear operator is a well-known and important problem in many areas of mathematics, and as such, Chapter 4 is expected to have an impact on a larger research community.

Summarizing, the variation from technical Chapters 2 and 3 on the one hand, to the more theoretical Chapter 4 on the other, shows that the applicant has a broad knowledge in the field of computational mathematics as well as good implementation and programming skills.

3. Mathematical content.

The mathematical results in the thesis seem correct, although due to the mentioned technical nature of especially Chapters 2 and 3, I did not inspect the validity each inequality that I encountered, leaving this to the referees of journals to which the various parts of this thesis have been, or will be, sent to.

The structuring of these results is adequate, although the reader is not assisted equally well at all points into what is about to be done. As an example, Section 1.2.3 gives information about Raviart-Thomas-Nédélec spaces. This information is correct, but it would be very helpful to read *why* these results are being given, if only by a single sentence. Since these spaces only appear again on page 42, where there they are redefined in (3.10) and moreover, only needed in *broken* form, it seems to me that Section 1.2.3 could be removed from the thesis without any consequences. As another example, the methods for which a posteriori error estimates are being developed in Chapter 2 are the so-called *interior penalty discontinuous Galerkin methods*. The reader is referred to references [38,39] (see page 14, line 5) but [39] is an unpublished manuscript and [38] is a book not available in Dutch libraries. It would have been helpful to find *in this thesis* more details (if only briefly) about this method such as, for instance, stability and a priori analysis.

The numerical experiments of Chapter 3 give abundant information. The results are very satisfactory and confirm the theory. As mentioned earlier, they prove the applicants insight in the methods and her ability to write nontrivial computer codes. Still, the representation of the results as the colorful Figures 3.7 to 3.21 has a minor flaw: the *same color* can correspond to *different values* that are being compared. For instance, red in the left picture of Figure 3.15 means $12 \cdot 10^{-7}$ whereas in the right picture is means $12 \cdot 10^{-6}$, a factor ten smaller. I stress that no false information is given, only that optical suggestion in many of the examples given, differs from the plain numerical facts.

The title of the thesis seems somewhat inappropriate: it is already mentioned by the applicant in the introduction (halfway page 10) that the thesis does not consider convection at all. The two model problems are the Laplace equation and the Heat equation, both in their simplest form without complicating coefficients. Even though I fully understand that the *mathematical analysis* as given in the thesis may only be possible for these simple model equations, it would have been nice to see at least one *numerical experiments* for a problem with convection, for which the methods, in the end, are being developed. Since this is not the case, I think that the title of the thesis could have been chosen to be more close to its factual content.

Finally, about Chapter 4. The applicant has chosen to study the *smallest singular value* σ_1 of a boundedly invertible linear operator $\gamma : V \to H$, or equivalently, the *operator norm* of γ^{-1}, in terms of the square root of the smallest *eigenvalue* λ_1 of the symmetric positive definite operator $\gamma^*\gamma : V \to V$. This is also how it is often done in the finite dimensional case, for matrices. For matrices, it is however also known that this squares the *condition number* of the problem, in a way that is very similar to solving *normal equations* in the least-squares context. For the latter, it is known that this unnecessarily complicates matters. Also in the present context, computing lower bounds it for may suffer from approximating steps much more than when the smallest singular value is addressed *directly*. Unfortunately, and contrary to linear algebra, singular values have not yet such prominent place in functional analysis. This is demonstrated also in this thesis, by Lemma 4.2.2, where the orthogonality of the *left singular vectors* is rediscovered, and also by the lack of references to the rather vast literature on (attempts to derive) lower bounds for smallest *singular values*.

The approach of the applicant in Chapter 4 is notwithstanding an interesting and creative mix of *priori-a posteriori inequalities* and the *complementarity technique*, and is quite original. It leads to good and often tight upper bounds of λ_1 and consequently, for σ_1. This is also demonstrated in the numerical experiments in Sections 4.3, 4.4, and 4.5.

But, also for this Chapter, one point of mild criticism: the applicant writes in the introduction on page 76 that the lower bounds on σ_1 in the literature [9,70,72,85,109] *do not guarantee that the computed approximation is really below the exact value.* In the Introduction, page 10 halfway, she claims that in this thesis, guaranteed lower bounds will be developed. But on page 82 halfway we read *The assumption (4.12) is crucial and cannot be guaranteed unless lower bounds on* λ_1 *and* λ_2 *are known.* Thus, we need a lower bound on λ_1 in order to arrive at ... a lower bound for λ_1. It is explained how to obtain such a lower bound, which is, to apply the Galerkin method: *since the Galerkin method is known to converge [15,16,31] with known speed, very accurate approximations of* λ_1 *and* λ_2 *can be computed.* After some more information, the section ends with the conclusion that *good confidence in the validity of (4.12)* is obtained. But, in my opinion, *good confidence* and *guarantees* are not the same, and thus, similar to references [9,70,72,85,109], also the work in Chapter 4 does not seem to lead to guaranteed lower bounds, and judgment of the literature [9,70,72,85,109] is better withheld.

4. Recommendation. My overall judgment of the thesis is positive. The candidate has carefully studied complicated material, extended existing results, and discovered and developed a new and interesting approach to the smallest singular value problem. She has proved to be able to perform independent original research in both theoretical and applied computational mathematics, as well as in computer programming. I therefore recommend that candidate will be awarded the promotion to PhD.

Jan Brandts, Utrecht, November 27, 2013.