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Habilitation thesis

speciality applied mathematics

presented by

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Title:

A POSTERIORI ERROR ESTIMATES, STOPPING CRITERIA, AND INEXPENSIVE IMPLEMENTATIONS

for error control and efficiency in numerical simulations

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Preface

This habilitation summarizes the works that I had a chance to be involved in as a "maître de conférences" (associate professor) at the Laboratoire Jacques-Louis Lions, Université Pierre et Marie Curie, Paris, and also, initially, as a postdoctoral fellow of the French National Center for Scientific Research in Orsay.

The main subject of this habilitation is the numerical analysis and to a lesser extent scientific calculation. The majority of the papers contain theoretical results: well-posedness analysis, convergence proofs, a priori and a posteriori error estimates, and proposition and study of adaptive algorithms. I was also involved in development of scientific calculation simulation codes.

Many of the results presented herein are closely related to, or motivated by, practical calculations and real-life problems. In my postdoctoral stay I collaborated with the HydroExpert society on simulations of flow and contaminant transport in the underground porous media, developing an adaptive simulation code. At the Université Pierre et Marie Curie, I was truly glad to have been involved in the project *A posteriori estimates for efficient calculations and error control in numerical simulations of porous media* in the framework of the French National Center for Scientific Research research project GNR MoMaS *Mathematical Modeling and Numerical Simulations for Nuclear Waste Repository Problems*. This project included interactions with the CEA (Commissariat à l'énergie atomique, the French nuclear energy research center). Finally, I have had a chance to collaborate with the IFP (the French Petroleum Institute) via the ERT project *Enhanced oil recovery and geological sequestration of* CO_2*: mesh adaptivity, a posteriori error control, and other advanced techniques*.

I believe sincerely that mathematics and in particular numerical analysis should be applied to real problems in order to advance the technological limits. Hopefully the results presented in this habilitation will help to do so...

Acknowledgements

My first acknowledgements go to all the members of the Laboratoire Jacques-Louis Lions. In particular, I am very much grateful to its director, Yvon Maday, who welcomed me with open arms. Laboratoire Jacques-Louis Lions is truly a great place to work, with perfect scientific conditions, a very stimulating environment, many various events taking place, an amazing number of people that I deeply appreciate both scientifically and humanly, and—which I value personally very much—an extremely friendly atmosphere.

I would like to thank very sincerely Roland Becker, Serge Nicaise, and Rüdiger Verfürth to have accepted to be my referees and for all their opinions expressed in the reports. And I am truly honored that Alexandre Ern, Raphaèle Herbin, Yvon Maday, Rolf Stenberg, and Zdeněk Strakoš have accepted to participate at my thesis committee.

My warmest personal thanks go to Alexandre Ern; for these hours, days, weeks, and months that we have spent together on the exciting walk along the edge between the known and unknown; for these many trials, fails, but also successes that we could celebrate at the end of a long way... Alexandre, thanks for everything and thanks also for reading this manuscript!

I am very much grateful to Christine Bernardi, Faker Ben Belgacem, and Adel Blouza. Thanks to them, I have started to discover the world of variational inequalities.

I am very glad to have had a chance to interact with all the people of the MoMaS research project; thanks to Linda El Alaoui, thanks to Annette Stephansen, thanks to Pascal Omnes, Christophe Le Potier, and Philippe Montarnal, and thanks to Jean Roberts and Jérôme Jaffré.

It was my personal pleasure to work on the ERT project with the IFP, the French Petroleum Institute. My note of gratitude goes to Roland Masson and Daniele Di Pietro in particular.

I feel very much enriched by all my visits in Austin. I would like to thank Gergina Pencheva, Todd Arbogast, Tim Wildey, Guangri Xue, and all the other people at the Center for Subsurface Modeling, for the countless discussions on mixed methods, multiscales, and mortars. My special personal thanks go to Mary Wheeler for all of the above but also for the visit to her ranch and the unforgettable wild boar hunting...

One of my intimacies are my feelings for my home country. It was an honor and a pleasure for me to work with Zdeněk Strakoš and Pavel Jiránek, until we have finally stopped the solver! And it is a joy for me to work with Vít Dolejší, on all that is discontinuous.

My especial warm thanks go to Barbara Wohlmuth for all the hours and days of exciting discussions, not only on mathematics after all.

I enjoyed my visit in Finland greatly. I would like to thank Rolf Stenberg for this experience, and, of course, mainly for the work on the Stokes problem. Also thanks to Antti Hannukainen, our programming guru.

I enjoyed truly a lot (and hopefully still will be doing so) our collaboration with Sorin Pop and Clément Cancès. Vivat the two-phase flows!

I am very grateful to Danielle Hilhorst for her support during my post-doc and for her constant encouragement. I owe a lot to Robert Eymard from whom I have learned a great deal. My thanks related to my beginnings go to everyone at HydroExpert; in particular to Lionel Demongodin for his support and to Marc Bonnet for all the discussions on the hydrological background. Also, thanks a lot to Libor Inovecký from Prague. We have spent a large portion of time on the programming concepts of the code TALISMAN (and a little bit on the guitar as well...). A special note of gratitude goes to everyone at the Technical University of Liberec, in particular Jiří Maryška, Jan Šembera, Otto Severýn, and Milan Hokr.

I have very warm remembrances for my stay in Japan with Mayan Mimura. This experience included not only programming with Matlab, reaction–diffusion systems, but the Japanese

lifestyle as well.

It is always a personal pleasure for me to discuss with Jean-François Maître. I wish I have his energy and enthusiasm when I reach his age!

I would like to thank particularly to Marie Postel for her kind help with proofreading of this manuscript.

I have fond memories of the CEMRACS 2007 research center and summer school. Thanks to the organizers! And thanks to the members of my student project, Mariana, Ibrahim, and Radek, for all the work we have done and for all the fun we had.

One of my biggest personal sources of happiness is the stimulus I get from my students. Thanks Nancy, thanks Carole, thanks Soleiman. And good luck for your theses!

I am honored and delighted to take part at the organization of the numerical analysis seminar at the Laboratoire Jacques-Louis Lions. I have learned a lot from Vivette Girault and Olivier Pironneau and express my gratitude to them for this opportunity.

One last iteration: thanks to all the secretaries in those various destinations. I could never have traveled without them: thanks to Connie Baxter, Tuula Donskoi, Lindsey Maddox, and Brit Steiner.

So here I am at the end. On my personal treasures. I would never have achieved this habilitation without the support of my fiancée Martina and her infinite understanding for my staying late at work, traveling on a conference, being abroad... And I would never be where I am without my family, and without my friends...

To Martina

To my parents

Contents

Chapter 1

Introduction

1.1 General introduction and terminology

A large number of environmental and physical phenomena is described by partial differential equations. Unfortunately, in the vast majority of cases, it is not possible to find the analytical, *exact solutions* of these equations. Then numerical methods, i.e., mathematically-based algorithms evaluated with the aid of computers, are used as simulation tools.

Except of very particular cases, in accordance with their conception, numerical methods only deliver *approximate solutions*, typically functions defined in some finite-dimensional spaces, different from the exact solutions. Then two extremely important questions are:

1. How large is the overall error between the exact and approximate solutions?
2. Where is the error localized?

Answers to these two questions may be crucial in building bridges and dams, constructing cars and planes, weather forecast, drilling oil and natural gas, depollution of soils and oceans, drugs conception, advanced health care techniques, population dynamics simulations, economic and financial predictions etc., as a decision is often taken on the basis of the numerical simulation result; cf., e.g., Ladevèze and Moës [112], Babuška and Oden [23], and Oden et al. [128]. Taking this reflection one step further, the ultimate goal is to design algorithms such that:

3. A precision, given before the simulation start, is attained at the end of the simulation (*error control*).
4. As small as possible amount of computational work is needed (*efficient calculation*).

We introduce below several themes allowing to contribute to the satisfaction of this goal: a posteriori error estimates, stopping criteria and adaptive discretizations, and inexpensive implementations.

1.1.1 A posteriori error estimates

Traditionally, the quality of numerical solutions is expressed with the aid of *a priori error estimates*. These estimates can be evaluated prior to the calculation and give bounds on the difference between the exact solution and the approximate solution, which is a function of some mesh-size constant (tending to zero with mesh refinement) and an unknown constant which depends on the exact solution. They are used to justify theoretically the numerical method

in question but they cannot be evaluated in general in practice and used in order to give an answer to the above questions and satisfy the above points.

A posteriori error estimates aim at giving bounds on the error between the known numerical approximation and the unknown exact solution that can be computed in practice, once the approximate solution is known, cf. Verfürth [161], Ainsworth and Oden [9], Babuška and Strouboulis [26], Neittaanmäki and Repin [122], Han [96], or Repin [141]. Thus, in principle, they might be used in order to answer the questions 1 and 2 above. Consequently, there is a hope to construct algorithms satisfying points 3 and 4 above.

One may formulate the following five properties describing an optimal a posteriori error estimate:

- **i)** deliver an upper bound on the error between the exact and approximate solutions which only uses the approximate solution and which can be fully, without the presence of any unknown quantities, evaluated (*guaranteed upper bound*);
- **ii)** give an expression for the estimated error locally, for example in each element of the computational mesh, and ensure that this estimate on the error represents a lower bound for the actual error, up to a generic constant (*local efficiency*);
- **iii)** ensure that the effectivity index, given as the ratio of the estimated and actual error, goes to one as the computational effort grows (*asymptotic exactness*);
- **iv)** guarantee the three previous properties independently of the parameters and of their variation (*robustness*);
- **v)** give estimators which can be evaluated locally (*small evaluation cost*).

Property **i)** allows to give a truly computable error upper bound, i.e., to answer the question 1 above. Property **ii)** enables to predict the error localization, i.e., to answer the question 2 above. Knowing where the error is, one can concentrate more effort in this part of the computational domain; typically, the mesh is refined in such parts, leading to the so-called concept of *adaptive mesh refinement*. Property **iii)** ensures the optimality of the upper bound; if the error is quite small and estimator predicts a large value, it may still satisfy property **i)** but is probably not too useful as it overestimates highly the error. Property **iv)** is one of the most important in practice. In real-life problems, parameters and coefficients (diffusivity, reactivity, convection, size of the nonlinearity, relative size of space and time scales) may vary over several degrees of magnitude; an estimator satisfying property **iv)** ensures that its results will be equally good in all situations. Finally, property **v)** guarantees that the evaluation cost will be much smaller than the cost required to obtain the approximate solution itself (recall that usually some kind of a global problem needs to be solved in order to obtain the approximate solution).

We give below in Section 2.1 the state of the art in a posteriori error estimates.

1.1.2 Stopping criteria and adaptive discretizations

A numerical algorithm typically involves several iterative procedures. As an example, for a nonlinear instationary problem, there is usually a loop over time steps, a linearization iteration, and, if an iterative algebraic solver is used, an algebraic solver iteration, cf. Szabó and Babuška [153], Quarteroni and Valli [137], Babuška and Strouboulis [26], Ern and Guermond [82], and Han [96]. Towards the satisfaction of the points 3 and 4 above, one may intend, at each moment of the calculation:

- **i)** distinguish and estimate separately the different error components (*error components*

identification and separation);

ii) classify the error components into two groups: *substantial error components* (crucial for the calculation, those errors which will always be present (e.g., spatial discretization error, temporal discretization error)) and *subsidiary error components* (side for the calculation, those errors which are in general made small or even zero for a sufficient number of iterations (e.g., linearization error, linear algebraic solver error));

iii) stop the different iterative algorithms whenever the corresponding subsidiary errors drop to the level at which they do not affect significantly the overall error (*stopping criteria*);

iv) adjust the calculation parameters (e.g., space meshes and time steps) such that the substantial errors are equally distributed and of comparable size (*error components equilibration*).

It is stated in Baxter and Iserles [31, p. 273], "The purpose of computation is not to produce a solution with least error but to produce reliably, robustly and affordably a solution which is within a user-specified tolerance." Therefore the substantial errors on the different stages should be in balance and the subsidiary errors small, see, e.g., Babuška [21], Han [95], Becker et al. [35], Ladevèze and Moës [113, 112], Ladevèze [110], Babuška and Oden [23], Oden et al. [128], Strakoš and Tichý [150], and Chaillou and Suri [61, 62]. In the present setting, satisfying the properties **i)**–**iv)** above will lead to efficient calculation allowing for error control in the sense of Section 1.1.

1.1.3 Implementations, relations between methods, and local postprocessing

As mentioned earlier, one of the central points in numerical simulations is the question of the efficiency of calculations. One numerical method may often be implemented in many different ways, leading to the same result in all cases. We call such implementations *equivalent implementations*. If one can find a way which is less expensive in terms of the computational cost than the other ones, one gains a lot in terms of efficiency. Typically, influencing the final matrix properties (symmetry, positive definiteness, number of unknowns, stencil (the number of nonzero entries per matrix row), condition number) is a way how to achieve an *inexpensive implementation*.

Different equivalent implementations of one numerical method are closely related to seemingly different formulations/different numerical methods which may be shown equivalent in the sense that the same result can be obtained at the end of the day; then we speak about *equivalent numerical methods*. Let us take the example of the vertex-centered finite volume method and of the finite element method. The first one is locally conservative by construction, whereas the second one is not. It, nevertheless, appears that, under certain conditions, these two methods are equivalent (the same result can be obtained at the end of the calculation). The equivalence relation then allows to reconstruct locally conservative fluxes also from the finite element method (such fluxes are not at the disposition at a first sight).

Some of these concepts are in fact closely related to techniques used in a posteriori error estimates. Herein, *local postprocessing*, i.e., local construction of new/improved approximations, plays a central role. In a posteriori error estimates, one typically postprocesses, by a local construction, conforming potentials and/or conforming, locally conservative fluxes. The terms *potential reconstruction* and *flux reconstruction* are also used.

Let us finally mention that the above techniques also allow for nontraditional a priori analyses.

1.2 List of papers of this habilitation

The papers forming this habilitation are organized into three different groups: papers in international peer-reviewed journals, papers submitted to international peer-reviewed journals (and one important paper currently in preparation), and short papers, notes, and conference proceedings.

The first group is formed by papers of regular length, published or accepted for publication in international peer-reviewed journals. The only exception is the paper [A3], which is a paper resulting from a student project carried out during the CEMRACS 2007 research center and summer school, which has been published in the *ESAIM: Proceedings* journal. I have included [A3] herein and not in the last group as this research is original, has not been published elsewhere, and the paper is of regular length. The papers in this group are referenced with the letter "A" at the beginning and form the basis of the habilitation.

The second group is formed by papers of regular length, submitted for publication to international peer-reviewed journals, and one paper currently in preparation. They are included here as, in my opinion, many important results are presented therein. The papers in this group are referenced with the letter "B" at the beginning.

The last, third, group is formed by short papers, notes, and conference proceedings. Typically, these papers served for announcement of ideas which have been developed later on in one of the papers of the first group. The papers in this group are referenced with the letter "C" at the beginning and I list them here for completeness only.

No paper listed below has been part of or is directly linked with my Ph.D. thesis.

After each paper, I give in brackets the page numbers where it is cited.

1.2.1 Papers in peer-reviewed journals

[A1] Ben Belgacem, F., Bernardi, C., Blouza, A., and Vohralík, M. A finite element discretization of the contact between two membranes. *M2AN Math. Model. Numer. Anal. 43*, 1 (2009), 33–52. [16, 18, 21, 42, 62, 63]

[A2] Ben Belgacem, F., Bernardi, C., Blouza, A., and Vohralík, M. On the unilateral contact between membranes. Part 1: Finite element discretization and mixed reformulation. *Math. Model. Nat. Phenom. 4*, 1 (2009), 21–43. [20, 21, 63]

[A3] Cheddadi, I., Fučík, R., Prieto, M. I., and Vohralík, M. Computable a posteriori error estimates in the finite element method based on its local conservativity: improvements using local minimization. *ESAIM Proc. 24* (2008), 77–96. [14, 16, 17, 28, 30, 38, 42, 63]

[A4] Cheddadi, I., Fučík, R., Prieto, M. I., and Vohralík, M. Guaranteed and robust a posteriori error estimates for singularly perturbed reaction–diffusion problems. *M2AN Math. Model. Numer. Anal. 43*, 5 (2009), 867–888. [16, 18, 38, 63]

[A5] El Alaoui, L., Ern, A., and Vohralík, M. Guaranteed and robust a posteriori error estimates and balancing discretization and linearization errors for monotone nonlinear problems. *Comput. Methods Appl. Mech. Engrg.* (2010). DOI 10.1016/j.cma.2010.03.024. [16, 18, 19, 43, 44, 45, 51, 54, 63, 66]

[A6] Ern, A., Stephansen, A. F., and Vohralík, M. Guaranteed and robust discontinuous Galerkin a posteriori error estimates for convection–diffusion–reaction problems. *J. Comput. Appl. Math. 234*, 1 (2010), 114–130. [16, 17, 18, 29, 31, 39, 40, 63]

[A7] Ern, A., and Vohralík, M. A posteriori error estimation based on potential and flux reconstruction for the heat equation. *SIAM J. Numer. Anal. 48*, 1 (2010), 198–223. [16, 18, 19, 20, 40, 46, 47, 48, 49, 51, 56, 63]

[A8] Eymard, R., Hilhorst, D., and Vohralík, M. A combined finite volume–finite element scheme for the discretization of strongly nonlinear convection–diffusion–reaction problems on nonmatching grids. *Numer. Methods Partial Differential Equations 26*, 3 (2010), 612–646. [20, 60, 61]

[A9] Hilhorst, D., and Vohralík, M. A posteriori error estimates for combined finite volume–finite element discretizations of reactive transport equations on nonmatching grids. *Comput. Methods Appl. Mech. Engrg.* (2010). DOI 10.1016/j.cma.2010.08.017. [16, 18, 19, 20, 49, 50, 51, 56, 63]

[A10] Jiránek, P., Strakoš, Z., and Vohralík, M. A posteriori error estimates including algebraic error and stopping criteria for iterative solvers. *SIAM J. Sci. Comput. 32*, 3 (2010), 1567–1590. [16, 17, 19, 35, 36, 37, 51, 53, 63, 66]

[A11] Vohralík, M. A posteriori error estimates for lowest-order mixed finite element discretizations of convection-diffusion-reaction equations. *SIAM J. Numer. Anal. 45*, 4 (2007), 1570–1599. [16, 18, 21, 29, 31, 32, 33, 38, 39, 40, 50, 62, 63]

[A12] Vohralík, M. Residual flux-based a posteriori error estimates for finite volume and related locally conservative methods. *Numer. Math. 111*, 1 (2008), 121–158. [16, 18, 21, 33, 38, 39, 50, 61, 63]

[A13] Vohralík, M. Guaranteed and fully robust a posteriori error estimates for conforming discretizations of diffusion problems with discontinuous coefficients. *J. Sci. Comput.* (2010). DOI 10.1007/s10915-010-9410-1. [16, 17, 25, 26, 27, 28, 29, 30, 42, 63]

[A14] Vohralík, M. Unified primal formulation-based a priori and a posteriori error analysis of mixed finite element methods. *Math. Comp. 79*, 272 (2010), 2001–2032. [16, 17, 21, 32, 33, 62, 63]

1.2.2 Papers submitted to peer-reviewed journals

[B1] Ben Belgacem, F., Bernardi, C., Blouza, A., and Vohralík, M. On the unilateral contact between membranes. Part 2: A posteriori analysis and numerical experiments. Preprint R10004, Laboratoire Jacques-Louis Lions, submitted for publication, 2010. [16, 18, 20, 21, 42, 43, 63]

[B2] Hannukainen, A., Stenberg, R., and Vohralík, M. A unified framework for a posteriori error estimation for the Stokes problem. Preprint R10016, Laboratoire Jacques-Louis Lions & HAL Preprint 00470131, submitted for publication, 2010. [16, 18, 40, 41, 42, 63]

[B3] Pencheva, G. V., Vohralík, M., Wheeler, M. F., and Wildey, T. Robust a posteriori error control and adaptivity for multiscale, multinumerics, and mortar coupling. Preprint R10015, Laboratoire Jacques-Louis Lions & HAL Preprint 00467738, submitted for publication, 2010. [16, 17, 19, 20, 33, 34, 35, 55, 63]

[B4] Vohralík, M. A posteriori error estimates, stopping criteria, and adaptivity for two-phase flows. In preparation, 2010. [16, 19, 20, 51, 52, 57, 63]

[B5] Vohralík, M., and Wohlmuth, B. I. Mixed finite element methods: implementation with one unknown per element, local flux expressions, positivity, polygonal meshes, and relations to other methods. Preprint R10031, Laboratoire Jacques-Louis Lions and HAL Preprint 00497394, submitted for publication, 2010. [20, 60, 66]

1.2.3 Short papers, notes, and conference proceedings

[C1] Ern, A., Nicaise, S., and Vohralík, M. An accurate **H**(div) flux reconstruction for discontinuous Galerkin approximations of elliptic problems. *C. R. Math. Acad. Sci. Paris 345*, 12 (2007), 709–712. [16, 17, 31, 63]

[C2] Ern, A., and Vohralík, M. Flux reconstruction and a posteriori error estimation for discontinuous Galerkin methods on general nonmatching grids. *C. R. Math. Acad. Sci. Paris 347*, 7-8 (2009), 441–444. [16, 17, 28, 31, 63]

[C3] Vohralík, M. A posteriori error estimates for finite volume and mixed finite element discretizations of convection–diffusion–reaction equations. *ESAIM Proc. 18* (2007), 57–69. [16, 18, 38]

[C4] Vohralík, M. A posteriori error estimation in the conforming finite element method based on its local conservativity and using local minimization. *C. R. Math. Acad. Sci. Paris 346*, 11–12 (2008), 687–690. [16, 17, 25, 26, 27, 28, 42, 63]

[C5] Vohralík, M. Two types of guaranteed (and robust) a posteriori estimates for finite volume methods. In *Finite Volumes for Complex Applications V*. ISTE and John Wiley & Sons, London, UK and Hoboken, USA, 2008, pp. 649–656. [16, 17, 28]

1.3 Main contributions of this habilitation

I associate here the papers, preprints, and notes of the three above lists with the three themes introduced in Section 1.1. In all the listings below, the works are sorted by date.

As described in the Preface, the majority of the papers of this habilitation contain theoretical results: well-posedness analysis, convergence proofs, a priori and a posteriori error estimates, and proposition and study of adaptive algorithms. Many of these results are, however, motivated or directly linked to practical demands in simulations of real-life problems. These include the simulation of underground nuclear waste disposals in the framework of the GNR MoMaS project *A posteriori estimates for efficient calculations and error control in numerical simulations of porous media* and the simulation of multiphase flows in the framework of the ERT project *Enhanced oil recovery and geological sequestration of* CO_2*: mesh adaptivity, a posteriori error control, and other advanced techniques*. Some of the papers also give algorithms from the developed scientific calculation simulation codes.

1.3.1 A posteriori error estimates

After my Ph.D. thesis, the primary focus of my research was the a posteriori analysis, cf. the introduction in Section 1.1.1. My contributions to this topic are the papers [A11, A12, A3, A1, A4, A6, A7, A14, A10, A5, A13, A9], the preprints [B1, B3, B2, B4], and the notes [C3, C1, C4, C5, C2]. I have, together with my collaborators, focused on development of a posteriori error estimates for various problems and various numerical methods, satisfying as much as possible the five optimal properties of Section 1.1.1. I have in particular worked intensively on estimates which are simultaneously guaranteed and robust, and this also for instationary and nonlinear problems. I have also worked on unified frameworks. To the best of my knowledge, such results are very rare in the literature or do not exist at all, cf. the state of the art in a posteriori error estimates given in Section 2.1 below. These contributions are the subject of Chapter 2.

Stationary linear problems

I have studied a stationary linear diffusion equation (the Laplace equation or the diffusion equation with a general inhomogeneous and anisotropic diffusion coefficient), discretized by the piecewise affine, continuous finite element method (cf. Ciarlet [67]), in [C4] and [A3, A13]. Similar results for the discontinuous Galerkin method are given in [C1, C2] and [A6] and for the cell- and vertex-centered finite volume methods in [C5] and [A13], respectively. The major idea of these developments goes back to the Prager–Synge equality, see Prager and Synge [136]. The first focus in these works was to obtain estimates satisfying the property **i)**, i.e., to ensure that the estimate gives a guaranteed upper bound on the error, without a presence of any unknown generic constant, so that the overall error in these different numerical discretizations can be controlled. Simultaneously, I put an emphasis to satisfy as much as possible the property **iii)** (the obtained effectivity indices typically range between 1.1 and 1.4). In addition, in [A13], I was able to give an estimate fully robust with respect to the discontinuities in the diffusion tensor, i.e., satisfying the property **iv)**. All the above estimates satisfy the properties **ii)** and **v)** of Section 1.1.1.

The work [A13] contains a systematic comparison of finite difference, piecewise affine finite element, and cell- and vertex-centered finite volume methods for a stationary linear diffusion problem with a general inhomogeneous and anisotropic diffusion coefficient. The relations/equivalences between these different numerical methods have been used in [A13] in order to present the a posteriori error estimates in a unified framework. In [C2], [A6], and partly in [A13], we were also able to take into account very general nonmatching grids. We give the details on all these developments in Section 2.2.1.

A unified framework for optimal a posteriori error estimates satisfying all the five optimal properties of Section 1.1.1 is given in [A14]. It is primarily developed for the different families and orders of the mixed finite element method, but it applies to any locally conservative method. This framework is presented in Section 2.2.2. Based on this framework, we have in the recent preprint [B3] achieved three main extensions. Firstly, different numerical methods (mixed finite element, discontinuous Galerkin, finite volume) can be used in different parts of the domain (*multinumerics*). Secondly, the *mortar technique* can be used. Lastly, the discretization can be done in the *multiscale setting*, allowing for the decomposition of the problem into h-scale subdomain problems and H-scale interface problems. Some of the family of estimators proposed in [B3] are robust with respect to the multiscale, i.e., with respect to the ratio H/h, under an assumption of sufficient regularity. These contributions are discussed in detail in Section 2.2.3; the use of these results for an adaptive strategy, following the idea in Wheeler and Yotov [175], is described in Sections 1.3.2 and 3.3.

The last work dedicated to the stationary linear diffusion equation is [A10]. In a discretization of such a problem, a system of linear algebraic equations needs to be solved. All the above results (as well as a vast majority of the results from the literature) are based on the assumption that this linear system has been solved exactly. This is often not the case in practice, as either direct solvers are used and then roundoff errors can be important, or iterative solvers are used and are stopped at some point, before reaching the (exact) convergence. The first result of [A10] are a posteriori error estimates which take into account the error in the solution of the algebraic linear system. Moreover, the (local) efficiency is proven. This means that our a posteriori error estimates are safe to be used for adaptive mesh refinement also in the presence of the algebraic error. This result is described in Section 2.2.4. It can be further used as a stopping criterion for iterative algebraic solvers, see Sections 1.3.2 and 3.1.

We have, together with my students, later studied the extension of the previous results

to the singularly perturbed reaction–diffusion case, while focusing on the robustness property **iv)**. We have in [A4] obtained estimates robust with respect to the size of the reaction term. This contribution is discussed in detail in Section 2.2.5. I have next, still in the stationary linear case, studied the convection–diffusion–reaction equation. The first results of [A11, A12] and [C3] satisfied the properties **i)**, **ii)**, (approximately) **iii)** and **v)** but not **iv)**. This missing robustness has been obtained in the collaboration [A6], upon replacing the energy norm by a norm consisting of the energy norm augmented by a dual norm of the convective derivative, following Verfürth [168]. These contributions are discussed in detail in Section 2.2.6.

The last extension in the stationary linear case is to the Stokes problem. We have carried it out in [B2]. A unified framework, comprising various conforming and conforming stabilized finite element methods, the discontinuous Galerkin method, the Crouzeix–Raviart nonconforming finite element method, the mixed finite element method, and a general class of finite volume methods, is developed therein, see Section 2.2.7.

Stationary variational inequalities

With my collaborators, I also had a chance to work on variational inequalities, namely on the contact between two membranes. We have first derived in [A1] a model for the contact between two membranes and performed its well-posedness analysis, as well as a priori error analysis. We have also derived herein a residual-based a posteriori error estimate. This estimate does not satisfy property **i)**. Moreover, property **ii)** is not satisfied optimally. We have been able to improve these two points and give guaranteed and locally efficient (up to a numerically negligible term) estimates in [B1]. These results are reported in Section 2.3.1.

Stationary nonlinear problems

We have studied a posteriori error estimates for stationary second-order monotone nonlinear problems in [A5]. We were able to achieve all the five optimal properties (the asymptotic exactness is only approximate); the derived estimates are in particular guaranteed and robust with respect to the size of the nonlinearity for the error measured as a dual norm of the residual. This result is described in Section 2.4.1. The use of these results for an adaptive stopping of the nonlinear solver is described in Sections 1.3.2 and 3.2.

Instationary linear problems

We have also, together with my collaborators, started work on instationary linear problems. We have, in particular, in [A7] developed a unified framework for a posteriori error estimation for the heat equation. Estimates giving a guaranteed upper bound on the error measured in the energy norm augmented by a dual norm of the time derivative, as well as error lower bounds, local-in-time but global-in-space, are derived under two simple conditions. It is then shown how to verify these conditions for the discontinuous Galerkin, various finite volume, and mixed finite element methods in space and the backward Euler scheme in time; extensions to conforming and nonconforming finite element spatial discretizations are also outlined. This result is described in Section 2.5.1.

In [A9], the previous result is extended to the instationary linear convection–diffusion–reaction equation. A guaranteed upper bound in the energy norm is obtained, and, using the approach of Verfürth [167], lower bound robust with respect to the convection dominance is shown for a dual norm. We refer to Section 2.5.2 for more details. Moreover, based on these results, an adaptive algorithm can be designed, cf. Sections 1.3.2 and 3.4.

Instationary nonlinear problems

Finally, the last result of [B4] is given for a two-phase flow model, a coupled system of instationary nonlinear convection–diffusion equations. It has been obtained in the framework of the ERT project collaboration with IFP, the French Petroleum Institute. In a unified setting as above, it gives a guaranteed upper bound on the error measured by the dual norm of the residual. The details are given in Section 2.6.1. Moreover, combing the approaches of [A10, A5, A7], an adaptive algorithm in the sense of Section 1.1.2 can be designed, see Sections 1.3.2 and 3.5.

1.3.2 Stopping criteria and adaptive discretizations

Another subject of my research in these last years, closely related to the a posteriori error estimates, were stopping criteria for linear and nonlinear iterative solvers and adaptive discretizations, cf. the introduction in Section 1.1.2. My contributions are contained in the papers [A10, A5, A9] and the preprints [B3, B4]. The goal is to derive stopping criteria satisfying as much as possible the four optimal properties of Section 1.1.2 and to design algorithms allowing for efficient calculation and error control in the sense of Section 1.1. These works include stopping criteria for linear algebraic solvers, stopping criteria for nonlinear solvers, error components equilibration in mortar discretizations, balancing of spatial and temporal errors in instationary problems, and also a fully adaptive discretization of an instationary nonlinear coupled system allowing to achieve a given precision. I, however, do not attempt to prove optimality of the algorithms, as it is the case, e.g., in Stevenson [149] or Cascon et al. [59] for model diffusion problems. These contributions are the subject of Chapter 3.

Stopping criteria for linear algebraic solvers

Stopping criteria for linear algebraic solvers, based on a posteriori error estimates and developing the ideas of, e.g., Babuška [21], Becker et al. [35], and Strakoš and Tichý [150], are derived in [A10]. Recall that our a posteriori error estimates enable to distinguish and estimate separately the different error components, in particular the error component corresponding to the discretization error (substantial component, stemming from the numerical scheme chosen and from the local mesh size) and the error component corresponding to the algebraic error (subsidiary component, stemming from the iterations of the algebraic solver). It turns out that as the iteration of an iterative algebraic solver continues, the algebraic error gets smaller and smaller, whereas the discretization error stagnates. In accordance with point **iii)** of Section 1.1.2, we suggest to stop the linear solver whenever the algebraic error does not affect significantly the overall error, i.e., when the algebraic error gets smaller than the discretization one. This can lead to important computational savings, as a great number of the linear algebraic solver iterations can typically be spared. We discuss this technique in Section 3.1.

Stopping criteria for nonlinear solvers

In a similar way as above, stopping criteria for nonlinear solvers (e.g., the Newton method or the fixed-point method) are derived in [A5], developing the ideas of Han [95] or Chaillou and Suri [61, 62]. An adaptive strategy, refining the computational mesh in places with increased error while stopping early the nonlinear solver, is outlined in Section 3.2.

Balancing the subdomain and interface errors in mortar discretizations

It is shown in [B3], on the basis of the a posteriori error estimates developed therein and following Wheeler and Yotov [175], how to derive an adaptive algorithm equilibrating the subdomain and mortar errors, so that an efficient calculation can be done in order to achieve a given precision. We present this algorithm in Section 3.3.

An adaptive discretization of an instationary convection–diffusion–reaction problem allowing to achieve a given precision

The a posteriori error estimates of [A7, A9] can be split into a part corresponding to the spatial error and into a part corresponding to the temporal error. Such an approach has already been advocated in, e.g., Picasso [133], Verfürth [165], or Bergam et al. [38], but our key result is that the ratio of the spatial and temporal errors is here not affected by any unknown constant. An adaptive algorithm equilibrating these two substantial error components can consequently be constructed. This algorithm, developed in [A9] for the instationary linear convection–diffusion–reaction equation, is presented in Section 3.4 along with some computational results.

An adaptive discretization of an instationary nonlinear coupled system allowing to achieve a given precision

Finally, an algorithm for stopping the algebraic and nonlinear solvers when the corresponding errors do not affect the overall error and equilibrating the space and time errors, developed on the basis of the a posteriori error estimates of [B4], is presented in Section 3.5. It allows for efficient calculation and error control in the sense of Section 1.1 for the two phase flow problem.

1.3.3 Implementations, relations between methods, and local postprocessing

The last general topic of my research after my Ph.D. were inexpensive implementations, relations between different numerical methods, and local postprocessing, cf. the introduction in Section 1.1.3. My contributions are contained in the papers [A2, A8], the preprints [B1, B5], and all the works on a posteriori analysis. The goal here is to achieve inexpensive implementations, develop unified frameworks, obtain improved approximations by local postprocessing, and present nontraditional a priori analyses. These contributions are the subject of Chapter 4.

Inexpensive implementations and relations between different numerical methods

The collaboration [B5] is a follow-up of the paper [170] which was a part of my Ph.D. thesis. It gives a framework for local elimination of the flux unknowns for lowest-order mixed finite element methods; consequently, these methods can be written with only one unknown per element, instead of one unknown per element and one unknown per side. The triple purpose of [B5] is to present a unified framework, comprising in particular the previous results [170] and Younès et al. [179], Chavent et al. [63], and Younès et al. [178], to show the closeness/equivalences of the mixed finite element and various finite volume-type methods, and to obtain an inexpensive implementation of the mixed finite element method leading to much smaller computational requirements. We give more details in Section 4.1.1.

Convergence analysis of the discretization of a degenerate parabolic convection–diffusion–reaction equation by a scheme combining cell-centered finite volumes and piecewise affine finite elements on nonmatching grids is the subject of the analysis of [A8]. This analysis relies on the

closeness/equivalence of these two methods. This paper is a follow-up of the paper [91] which was a part of my Ph.D. thesis and it builds upon the approach of Eymard et al. [87, 88, 90]; its main results are described in Section 4.1.2.

Improvement of approximate solutions by local postprocessing

The cell-centered finite volume method leads to approximations that are only piecewise constant in the mesh cells. This may not be sufficient in many cases. We in [A12] introduce a locally postprocessed approximation, yielding a piecewise parabolic approximate solution. This postprocessing is in fact the basis of the a posteriori error estimates of [A12]. We describe in Section 4.2.1 in details this postprocessing and present a result of [A12] giving an a priori error estimate for this postprocessing under sufficient regularity of the weak solution and a convergence result under the minimal regularity of the weak solution.

The mixed finite element method is usually analyzed in the dual mixed formulation framework relying on the Babuška [20]–Brezzi [46] inf–sup condition. We present in Section 4.2.2 a new a priori analysis of the mixed finite element method, relying on a local postprocessing, the primal weak formulation, and the discrete Friedrichs inequality. This result has been derived in [A14]; the local postprocessing is that of [A11, Section 4.1], Arnold and Brezzi [19], and Arbogast and Chen [13]. In particular, the uniform discrete inf–sup condition can be completely avoided and both a priori and a posteriori analyses can be done in a unified setting.

We have in [A1] derived a finite element method for the discretization of the contact between two membranes. The method proposed in this reference, however, had a rather increased number of unknowns; there was, in particular, a discrete unknown for the approximation of the action of one membrane on the other. The approach of [A2] and [B1] presents an equivalent formulation with the unknowns reduced to the approximations of the displacements of the two membranes only; an accurate action of one membrane on the other is then recovered by a local postprocessing. An a priori error estimate for this postprocessed approximation is also given. We present the details in Section 4.2.3.

In all the works mentioned in the part on a posteriori error analysis for nonconforming locally conservative methods in Section 1.3.1, a notion of a potential reconstruction appears. Such a reconstruction is of an independent interest; the methods in question deliver a discontinuous potential and the present one can be used in place of it. We present this general idea in Section 4.2.4. Similarly, in all the works mentioned in the part on a posteriori error analysis for conforming or discontinuous Galerkin methods in Section 1.3.1, a notion of a locally conservative flux reconstruction appears. This reconstruction is once again of an independent interest and we present it in Section 4.2.5.

Chapter 2

A posteriori error estimates

The purpose of this chapter is to give a posteriori error estimates satisfying as much as possible and as well as possible the five optimal properties of Section 1.1.1. In particular, all the estimates presented below, for various problems and methods, rigorously satisfy the guaranteed upper bound and are often robust with respect to diffusion inhomogeneities and anisotropies, convection or reaction dominance, size of the nonlinearity, and/or final simulation time. To the best of my knowledge, guaranteed and simultaneously robust a posteriori error estimates have not been established elsewhere before. I also focused on concentrating the analyses for different numerical methods into unified frameworks.

2.1 State of the art

A posteriori error estimates, in particular for the discretization of the Laplace equation by the finite element method, have received an enormous attention in the literature. Several main branches of a posteriori estimates have evolved during the last decades.

Explicit *residual estimates*, initiated by Babuška and Rheinboldt in [25] and presented in detail in Verfürth [161], are probably the most popular amongst numerical analysts. A rigorous mathematical theory exists, showing that they fulfill the desirable properties **i)**, **ii)**, **iv)**, and **v)** of Section 1.1.1. However, up to very rare exceptions, such as the works of Carstensen and Funken [53], Carstensen and Klose [56], or the modified approach of Veeser and Verfürth [157], the property **i)** is not satisfied in the strict sense, since one has a computable upper bound up to an unknown multiplicative constant. This constant is independent of the unknown solution and of the mesh size, but the estimate is only *reliable* and not guaranteed. Note that in particular studying the property **iii)** loses sense in this case.

The *equilibrated residual method*, cf. Ainsworth and Oden [9], removes the above drawbacks under the condition that local infinite-dimensional problems can be solved. This is hardly doable in practice and hence one has to approximate the solutions of these problems, leading to the loss of the guaranteed upper bound and increased computational cost. It can, however, be modified by replacing the infinite-dimensional problems by finite-dimensional ones while introducing a supplementary term only dependent on the data (the so-called data oscillation term), following Ainsworth [5].

Averaging estimates as the celebrated Zienkiewicz–Zhu one, see [180], are easy to compute, often fulfill the property **iii)**, but systematically fail with the property **i)** in the strict (guaranteed) sense. They can, however, be shown to satisfy the property **ii)**, see, e.g., Carstensen [51, 52].

Functional a posteriori error estimates, see Neittaanmäki and Repin [122] and Repin [141] and the references therein, satisfy the property **i)** by construction. It is, however, difficult for them to simultaneously satisfy the property **iii)** and **v)**; moreover, they are not robust (they do not fulfill the property **iv)**).

Other classes of a posteriori error estimates are widely used in practice, such as *hierarchical estimates*, cf. Bank and Smith [27], or *geometric a posteriori error estimates*, cf., e.g., Castro-Díaz et al. [60] or Frey and Alauzet [93].

The results presented below fall into the category of so-called *equilibrated fluxes estimates*, whose main ideas can be traced back to the Prager–Synge equality [136] and the hypercircle method, cf. Synge [152]. Estimates of this kind can be found in Ladevèze [109], Ladevèze and Leguillon [111], Repin [139], Destuynder and Métivet [75], Luce and Wohlmuth [118], Ainsworth [5], Vejchodský [158], Korotov [108], or Braess and Schöberl [44], see also Haslinger and Hlaváček [97], Vacek [154], Nečas and Hlaváček [120], Hlaváček et al. [100], and Fierro and Veeser [92]. They have also recently been shown robust with respect to the polynomial degree by Braess et al. in [43]. This distinguishes them from the other classes of estimates.

The differences between the various types of estimates become more important in the robustness property **iv)** for singularly perturbed problems. Not many robustness results were proven, and this mostly for the residual estimates. For the diffusion case with discontinuities in the diffusion coefficient, let us cite Dörfler and Wilderotter [80], Bernardi and Verfürth [41], Petzoldt [131], Ainsworth [4], or Chen and Dai [64]. All these estimates are, however, based on the "monotonicity around vertices" condition on the distribution of the diffusion coefficient (see [41, Hypothesis 2.7]) or a similar assumption. For the reaction–diffusion case, Verfürth [164] was able to obtain robust estimates in the energy norm. Similar results were obtained by Ainsworth and Babuška [7] and Grosman in [94] for the equilibrated residual method; neither of these bounds is guaranteed. In the convection–diffusion–reaction case, a robust result was obtained by Verfürth [168] upon augmenting the energy norm by the dual norm of the convective derivative. This result was extended to the discontinuous Galerkin case by Schötzau and Zhu [146]. An alternative approach for a different norm is pursued by Sangalli [145]; once again, neither of these bounds is guaranteed.

In the last years, there has been a vivid increase of various extensions and applications of a posteriori error estimates. Estimates for the Stokes problem have been derived in, e.g., Verfürth [159, 160], Dari et al. [71], Houston et al. [101], Dörfler and Ainsworth [79], Repin and Stenberg [142], or Becker et al. [33]. Estimates for multiscale, multinumerics, or mortar coupling have been derived in, e.g., Wohlmuth [176, 177], Belhachmi [36], Bergam et al. [37], Aarnes and Efendiev [1], Larson and Målqvist [115], and Creusé and Nicaise [70]. Algebraic error a posteriori error estimates and stopping criteria for iterative algebraic solvers have been derived in Becker et al. [35], Patera and Rønquist [129], Arioli et al. [18], Arioli and Loghin [17], Picasso [134], and Silvester and Simoncini [147]. For a posteriori error estimates for variational inequalities, we cite in particular Hlaváček et al. [100], Ainsworth [10], Chen and Nochetto [65], Veeser [155], Nochetto et al. [127], Hild and Nicaise [99], Braess et al. [42], and Weiss and Wohlmuth [174]. Finally, for nonlinear problems and linearization error estimators, let us quote Pousin and Rappaz [135], Han [95], Picasso [132], Verfürth [161], Liu and Yan [117], Veeser [156], Carstensen and Klose [56], Han [96], Carstensen et al. [57], Chaillou and Suri [61, 62], and Diening and Kreuzer [76].

Lately, a posteriori error estimates have also been derived for linear and nonlinear instationary problems. Let me cite in particular the works of Picasso [133], Verfürth [165], and Bergam et al. [38], where residual-based a posteriori error estimates for conforming finite elements and linear problems have been derived. I also mention Makridakis and Nochetto [119], Lakkis and

Makridakis [114], and de Frutos et al. [73] for the so-called elliptic reconstruction technique allowing for optimal error estimates in higher order norms for conforming finite elements. A posteriori error estimates based on flux reconstruction have been presented by Repin in [140], whereas Babuška and Ohnimus [24], Babuška et al. [22], and Strouboulis et al. [151] were able to extended to the heat equation in a conforming setting various estimators for elliptic problems. Extensions to nonconforming methods are given in, e.g., Nicaise and Soualem [123] or Cascón et al. [58]. Much less work has been done on nonlinear instationary problems; I quote, in particular, Nochetto et al. [124, 125, 126], Verfürth [162, 163, 166], Ladevèze and Moës [113, 112], Ladevèze [110], and Akrivis et al. [12].

To the best of my knowledge, a posteriori error estimates satisfying all the five optimal properties of Section 1.1.1 do not exist yet. Unified analyses and unified frameworks are also quite rare; I cite, in particular, Ainsworth and Oden [8], Ainsworth [5], Carstensen [52, 55], Carstensen et al. [54], and Kim [104, 105]. These two points also constitute my biggest motivation.

2.2 Stationary linear problems

2.2.1 Pure diffusion equation: guaranteed estimates

Let us consider the model second-order elliptic problem

$$-\nabla\cdot(\mathbf{S}\nabla p) = f \qquad \text{in } \Omega, \tag{2.1a}$$

$$p = 0 \qquad \text{on } \partial\Omega, \tag{2.1b}$$

where $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, is a polygonal (polyhedral) domain (open, bounded, and connected set), $\mathbf{S}$ is a symmetric, bounded, and uniformly positive definite tensor, and $f \in L^2(\Omega)$. The weak formulation consists in finding $p \in H^1_0(\Omega)$ such that

$$(\mathbf{S}\nabla p, \nabla\varphi) = (f, \varphi) \qquad \forall \varphi \in H^1_0(\Omega). \tag{2.2}$$

I present the a posteriori error estimates here quite in detail. I do so in view of the simplicity of the model problem (2.1a)–(2.1b) and also to highlight the main ideas and building principles that will be reused for more complicated problems below. I start with conforming lowest-order discretizations in the section below and then pass to a unified framework in the subsequent section.

Conforming discretizations

Let us consider the discretization of (2.2) by the lowest-order finite element method. It reads: find $p_h \in X^0_h$ such that

$$(\mathbf{S}\nabla p_h, \nabla\varphi_h) = (f, \varphi_h) \qquad \forall \varphi_h \in X^0_h. \tag{2.3}$$

Here X^0_h is the space of continuous, piecewise affine functions over a simplicial mesh $\mathcal{T}_h$ of Ω, equal to 0 on $\partial\Omega$.

I have in [C4] proposed a guaranteed a posteriori error estimate for the energy error between the (unknown) weak solution p of (2.2) and the finite element approximate solution p_h of (2.3). Recall that the energy error is given by

$$|||p - p_h||| := \|\mathbf{S}^{\frac{1}{2}}\nabla(p - p_h)\|. \tag{2.4}$$

Let $\mathcal{D}_h$ be a dual mesh to the simplicial mesh $\mathcal{T}_h$, formed by dual volumes around each vertex of the mesh $\mathcal{T}_h$ (we refer to Figure 2.1, left, for an example and to [A13, Section 2.1] for the

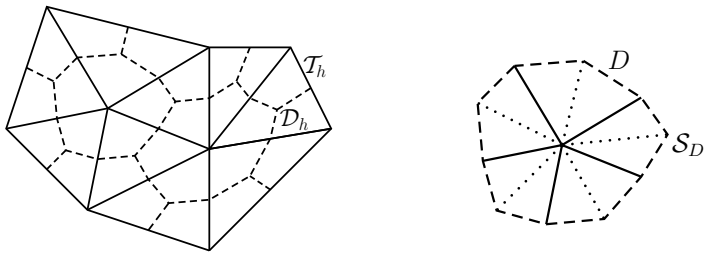

Figure 2.1: Original simplicial mesh $\mathcal{T}_h$ and an associated dual mesh $\mathcal{D}_h$ (left) and the fine simplicial mesh $\mathcal{S}_D := \mathcal{S}_h|_D$ of a dual volume $D \in \mathcal{D}_h$ (right)

details). Divide $\mathcal{D}_h$ into $\mathcal{D}_h^{\text{int}}$, containing the dual volumes associated with the interior vertices, and $\mathcal{D}_h^{\text{ext}}$, containing the dual volumes associated with the boundary vertices. Suppose for simplicity that $\mathbf{S}$ and f are piecewise constant on $\mathcal{T}_h$. Then we have, see [C4, Theorem 3.2] or [A13, Theorem 4.5] (we refer to Luce and Wohlmuth [118] for a closely related result and to [136, 152, 109, 97, 154, 120, 111, 100, 139, 75, 5, 158, 108, 44, 43] for similar ideas):

Theorem 2.2.1 (Guaranteed estimates for the diffusion problem (2.1a)–(2.1b) and the finite element discretization (2.3))**.** *Let p be the solution of (2.2) and p_h the solution of (2.3). Let a vector field $\mathbf{t}_h \in \mathbf{H}(\text{div}, \Omega)$ be arbitrary but such that*

$$(\nabla\cdot\mathbf{t}_h, 1)_D = (f, 1)_D \qquad \forall D \in \mathcal{D}_h^{\text{int}}. \tag{2.5}$$

Then

$$|||p - p_h||| \le \left\{ \sum_{D\in\mathcal{D}_h} (\eta_{\text{R},D} + \eta_{\text{DF},D})^2 \right\}^{\frac{1}{2}},$$

where the diffusive flux estimator *is given by*

$$\eta_{\text{DF},D} := \|\mathbf{S}^{\frac{1}{2}}\nabla p_h + \mathbf{S}^{-\frac{1}{2}}\mathbf{t}_h\|_D \qquad D \in \mathcal{D}_h, \tag{2.6}$$

and the residual estimator *is given by*

$$\eta_{\text{R},D} := m_{D,\mathbf{S}}\|f - \nabla\cdot\mathbf{t}_h\|_D \qquad D \in \mathcal{D}_h, \tag{2.7}$$

with the weighting coefficient

$$m_{D,\mathbf{S}} := C_{\text{P},D}^{\frac{1}{2}} \frac{h_D}{c_{\mathbf{S},D}^{\frac{1}{2}}} \quad D \in \mathcal{D}_h^{\text{int}}, \qquad m_{D,\mathbf{S}} := C_{\text{F},D,\partial\Omega}^{\frac{1}{2}} \frac{h_D}{c_{\mathbf{S},D}^{\frac{1}{2}}} \quad D \in \mathcal{D}_h^{\text{ext}}, \tag{2.8}$$

where h_D is the diameter of the dual volume D, $c_{\mathbf{S},D}$ is the smallest eigenvalue that $\mathbf{S}$ takes on D, and $C_{\text{P},D}$ and $C_{\text{F},D,\partial\Omega}$ are, respectively, the constants from the Poincaré (A.1) and the Friedrichs (A.2) inequalities.

We give here the proof of this theorem, as it is very simple and as we find it quite instructive.

Proof. The proof is divided into two steps.

Step 1 (*Characterization of the energy error*).

We first show that

$$|||p - p_h||| = \inf_{\mathbf{t}\in\mathbf{H}(\text{div},\Omega)} \sup_{\varphi\in H_0^1(\Omega),\, |||\varphi|||=1} \{|(f - \nabla\cdot\mathbf{t}, \varphi)| + |(\mathbf{S}\nabla p_h + \mathbf{t}, \nabla\varphi)|\}. \tag{2.9}$$

Notice that

$$|||p-p_h||| = \left(\mathbf{S}\nabla(p-p_h), \frac{\nabla(p-p_h)}{|||p-p_h|||}\right)$$

by (2.4) and the symmetry of $\mathbf{S}$. Define $\varphi := (p-p_h)/|||p-p_h|||$ and note that $\varphi \in H^1_0(\Omega)$. Thus, we immediately have $(\mathbf{S}\nabla p, \nabla\varphi) = (f,\varphi)$ by (2.2). Using this we obtain, for an arbitrary vector field $\mathbf{t} \in \mathbf{H}(\mathrm{div},\Omega)$, employing the Green theorem,

$$\begin{aligned}(\mathbf{S}\nabla(p-p_h),\nabla\varphi) &= (f,\varphi) - (\mathbf{S}\nabla p_h,\nabla\varphi) = (f,\varphi) - (\mathbf{S}\nabla p_h + \mathbf{t},\nabla\varphi) + (\mathbf{t},\nabla\varphi)\\ &= (f - \nabla\cdot\mathbf{t},\varphi) - (\mathbf{S}\nabla p_h + \mathbf{t},\nabla\varphi)\\ &\le |(f-\nabla\cdot\mathbf{t},\varphi)| + |(\mathbf{S}\nabla p_h + \mathbf{t},\nabla\varphi)|.\end{aligned}$$

From here, it is enough to note that $|||\varphi||| = 1$ and that $\mathbf{t} \in \mathbf{H}(\mathrm{div},\Omega)$ was chosen arbitrary to conclude that the right-hand side term of (2.9) is an upper bound on the left-hand side one. For the converse estimate, it suffices to set $\mathbf{t} = -\mathbf{S}\nabla p$ and to use (2.2), the Cauchy–Schwarz inequality, and the fact that $|||\varphi||| = 1$, cf. [C4, Theorem 2.1] or [A13, Theorem 4.1].

Step 2 (*Bounding the negative norm* (2.9) *using the local conservation property* (2.5)).

We now bound the right-hand side of (2.9). To this purpose, choose a vector field $\mathbf{t}_h \in \mathbf{H}(\mathrm{div},\Omega)$ satisfying (2.5) as $\mathbf{t}$ in (2.9). Let $D \in \mathcal{D}_h^{\mathrm{int}}$ and denote by φ_D the mean value of φ over D, $\varphi_D := (\varphi,1)_D/|D|$, where $|D|$ is the measure of D. Then, using (2.5), the Poincaré inequality (A.1), the Cauchy–Schwarz inequality, and the definition (2.4) of the energy norm,

$$|(f-\nabla\cdot\mathbf{t}_h,\varphi)_D| = |(f-\nabla\cdot\mathbf{t}_h,\varphi-\varphi_D)_D| \le \eta_{\mathrm{R},D}|||\varphi|||_D.$$

We cannot use a similar approach also for $D \in \mathcal{D}_h^{\mathrm{ext}}$ since there is no local conservativity assumed on these volumes (recall that (2.5) is only supposed to hold for $D \in \mathcal{D}_h^{\mathrm{int}}$). On the other hand, however, $\varphi = 0$ on $\partial D \cap \partial\Omega$, whence

$$|(f-\nabla\cdot\mathbf{t}_h,\varphi)_D| \le \eta_{\mathrm{R},D}|||\varphi|||_D$$

for each $D \in \mathcal{D}_h^{\mathrm{ext}}$, using the Friedrichs inequality (A.2), the Cauchy–Schwarz inequality, and the definition (2.4) of the energy norm. Finally, $|(\mathbf{S}\nabla p_h + \mathbf{t}_h,\nabla\varphi)_D| \le \eta_{\mathrm{DF},D}|||\varphi|||_D$ is immediate using the Cauchy–Schwarz inequality. We thus come to

$$|||p-p_h||| \le \sum_{D\in\mathcal{D}_h} (\eta_{\mathrm{R},D} + \eta_{\mathrm{DF},D})|||\varphi|||_D.$$

Hence, it now suffices to use the Cauchy–Schwarz inequality and to notice that $|||\varphi||| = 1$ in order to conclude the proof. □

Remark 2.2.2 (Flux reconstruction for the diffusion problem (2.1a)–(2.1b))**.** *We will call the vector field* $\mathbf{t}_h$ *from Theorem 2.2.1 an equilibrated* flux reconstruction*. The equilibration is here meant in two senses. Firstly, the* side fluxes *of* $\mathbf{t}_h$ *over the sides* σ *of the mesh* $\mathcal{D}_h$ *(and* $\mathcal{T}_h$*), i.e., the quantities* $\langle \mathbf{t}_h\cdot\mathbf{n}_\sigma, 1\rangle_\sigma$ *with* $\mathbf{n}_\sigma$ *the unit normal vector of* σ*, are* univalued*, the same for the two elements which share the given side* σ*. Secondly,* $\mathbf{t}_h$ *is by* (2.5) locally conservative*, on the mesh* $\mathcal{D}_h$*.*

In order to use the estimate of Theorem 2.2.1 in practice, we need a way to construct a flux reconstruction $\mathbf{t}_h$ satisfying the condition (2.5). For this purpose, we first construct a fine simplicial mesh $\mathcal{S}_h$, a submesh (conforming refinement) of both the original simplicial mesh $\mathcal{T}_h$ and of the dual mesh $\mathcal{D}_h$, see Figure 2.1, right. We then specify $\mathbf{t}_h$ in a finite-dimensional

subspace of $\mathbf{H}(\mathrm{div},\Omega)$, defined over the mesh $\mathcal{S}_h$. We choose for this purpose the lowest-order Raviart–Thomas [138] space or its three-dimensional equivalent of Nédélec [121]. These spaces are typically used in the mixed finite element method, cf. Brezzi and Fortin [47] or Roberts and Thomas [143].

A simple construction of the flux reconstruction $\mathbf{t}_h$ is suggested in [C4]. It consists in directly prescribing the degrees of freedom of $\mathbf{t}_h$ (the normal fluxes/components over the sides of the mesh $\mathcal{S}_h$) by

$$\mathbf{t}_h\cdot\mathbf{n}_\sigma := -\{\!\{\mathbf{S}\nabla p_h\cdot\mathbf{n}_\sigma\}\!\} \tag{2.10}$$

for all sides σ of the mesh $\mathcal{S}_h$. Here, $\{\!\{\cdot\}\!\}$ is the (arithmetic) averaging operator. The flux reconstruction $\mathbf{t}_h$ is in this case constructed from the approximate solution flux $-\mathbf{S}\nabla p_h$ by simple averaging of the normal components over the sides of the mesh $\mathcal{S}_h$. It turns out that this construction yields (2.5) (see [A13, Section 4.3] and the references therein). This construction can be shown locally efficient, see below, but, except in one space dimension, it leads to effectivity indices not close to the optimal value of one. It was the subject of [A3] to identify the reason for this fact and to suggest a remedy. The main idea is to use the averaging construction (2.10) only on those sides of the mesh $\mathcal{S}_h$ which lie on the boundary ∂D of a dual volume $D \in \mathcal{D}_h^{\mathrm{int}}$. This is sufficient for (2.5) to hold. The remaining degrees of freedom of $\mathbf{t}_h$ are then determined while solving some local discrete minimization problems in each dual volume $D \in \mathcal{D}_h$, see [A3, Section 3].

Two other constructions of $\mathbf{t}_h$ are proposed in [A13]. It turns out that the best results are obtained when $\mathbf{t}_h$ is a solution of local Neumann problems by the mixed finite element method, see [A13, Section 4.3.4]. This can be viewed as a generalization of the idea going back to Bank and Weiser [28] and, in its present form, it was proposed in [C2]. In [A13], all the above constructions of $\mathbf{t}_h$ are discussed in detail. Also, through the equivalences/close relations between the different classical numerical methods, Theorem 2.2.1 is extended in [A13] to the cell- and vertex-centered finite volume methods and to the finite difference method. The relations of the above estimate to the residual, equilibrated residual, averaging, functional, and other equilibrated fluxes estimates is discussed in [A13, Section 4.4]. Extensions to general inhomogeneous Dirichlet and Neumann boundary conditions are given in [C5].

An important and mathematically much more involved result is to show that the estimates of Theorem 2.2.1 are also locally efficient. This result is given in [A13] for the different constructions of the flux reconstruction $\mathbf{t}_h$ discussed above (see Theorems 5.1 and 5.5 in this reference). These results may be summarized as follows:

Theorem 2.2.3 (Local efficiency of the estimates for the diffusion problem (2.1a)–(2.1b) and the finite element discretization (2.3))**.** *For all $D \in \mathcal{D}_h$, there holds*

$$\eta_{\mathrm{DF},D} \le C C_{\mathbf{S},D}^{\frac{1}{2}} c_{\mathbf{S},D}^{-\frac{1}{2}} |||p-p_h|||_D, \tag{2.11a}$$

$$\eta_{\mathrm{R},D} \le C C_{\mathbf{S},D}^{\frac{1}{2}} c_{\mathbf{S},D}^{-\frac{1}{2}} |||p-p_h|||_D, \tag{2.11b}$$

where the constant C depends only on the space dimension d and on the shape regularity parameter of the mesh $\mathcal{S}_h$ and where $c_{\mathbf{S},D}$ is the smallest eigenvalue that $\mathbf{S}$ takes on D and $C_{\mathbf{S},D}$ is the largest eigenvalue that $\mathbf{S}$ takes on D.

The proof has two main steps. Firstly, we show that for any of the above constructions of the flux reconstruction $\mathbf{t}_h$, our estimates are in each dual volume smaller or equal to the classical residual estimates. The proof consists in using the way how the flux reconstruction $\mathbf{t}_h$ was constructed from the approximate flux $-\mathbf{S}\nabla p_h$. The main technical tools in the case of the

construction of $\mathbf{t}_h$ by (2.10) is the mapping to a reference element, by the Piola transformation as we are working with $\mathbf{H}(\mathrm{div},\Omega)$-conforming vectors, properties of Raviart–Thomas–Nédélec spaces, equivalence of norms on finite-dimensional spaces, and scaling arguments. The tools in the case of the construction of $\mathbf{t}_h$ by the mixed finite element solution of local Neumann problems, see [A13, proof of Theorem 5.5], are the use of local postprocessing of the mixed finite element solution, following [A11, Section 4.1], Arnold and Brezzi [19], and Arbogast and Chen [13], the Green theorem, the Cauchy–Schwarz inequality, the discrete Poincaré and Friedrichs inequalities, see Section A.2 below or [169], and the inverse inequality. This last inequality typically states that $\|\nabla v_h\|_K \leq C h_K^{-1} \|v_h\|_K$ for a polynomial v_h; here h_K is the diameter of the element K and C is a generic mesh-size-independent constant (see, e.g., Quarteroni and Valli [137, Proposition 6.3.2]).

In the second step, see [A13, proof of Theorems 5.1 and 5.4], the techniques of Verfürth [161] are employed. Firstly, element and edge bubble functions are introduced. These are polynomials which are such that they are nonzero only in the interior of a given simplex or a given side. With the help of these bubble functions, boundary terms, arising from the integration by parts of the Green theorem, can be discarded. Then once again mappings to a reference element, equivalence of norms on finite-dimensional spaces (recall that all the approximate solution, the data, and the bubble functions are polynomials), and scaling arguments are needed. The last ingredients in the lower bound proofs are the definition (2.2) of the weak solution, the Green theorem, the Cauchy–Schwarz inequality, definition (2.4) of the energy norm, and the inverse inequality.

Remark 2.2.4 (Robustness with respect to the discontinuities in $\mathbf{S}$ using harmonic averaging)**.** *One of the key results of [A13] is that it is possible to construct a flux reconstruction* $\mathbf{t}_h$ *such that the factors* $C_{\mathbf{S},D}^{\frac{1}{2}}/c_{\mathbf{S},D}^{\frac{1}{2}}$ *in* (2.11a)–(2.11b) *vanish. Crucially,* no "monotonicity around vertices" condition *on the distribution of the diffusion coefficient as that of [41, Hypothesis 2.7] or those of [80, 131, 4, 64]* is necessary here*, see Theorem 5.1 in [A13]. The main argument is to notice that, following [A6] (cf. also the preprint [84]), this* robustness with respect to the inhomogeneities in $\mathbf{S}$ *can be achieved whenever* harmonic averaging *is used both in the* numerical method *and in the* construction of $\mathbf{t}_h$*.*

Remark 2.2.5 (Robustness with respect to the discontinuities in $\mathbf{S}$ in a dual norm)**.** *Consider, instead of* (2.4)*, the* dual norm of the residual

$$|||p-p_h|||_{\#} := \sup_{\varphi \in H_0^1(\Omega)\setminus\{0\}} \frac{(\mathbf{S}\nabla(p-p_h),\nabla\varphi)}{\|\nabla\varphi\|} \tag{2.12}$$

as the error measure. Note that $|||p-p_h|||_{\#} = |||p-p_h|||$ *whenever* $\mathbf{S}$ *is constant and scalar but that* $|||p-p_h|||_{\#}$ *and* $|||p-p_h|||$ *are different in general. A guaranteed upper bound similar to that of Theorem 2.2.1 has been proved in [A13, Corollary 4.6] for this error measure. More importantly, a lower bound* robust with respect to *both the* inhomogeneities *and* anisotropies in $\mathbf{S}$ *is proven in [A13, Theorem 5.4 and Corollary 5.6].*

We now present some numerical results. As a first example, we show in Figure 2.2, left, the estimated and actual energy errors and the two estimators $\eta_{\mathrm{DF}} := \{\sum_{D\in\mathcal{D}_h} \eta_{\mathrm{DF},D}^2\}^{\frac{1}{2}}$ and $\eta_{\mathrm{R}} := \{\sum_{D\in\mathcal{D}_h} \eta_{\mathrm{R},D}^2\}^{\frac{1}{2}}$ for a model example in one space dimension, cf. [A13, Section 7.1.1]. Note that, as predicted by the theory, the estimate is bigger than or equal to the error, i.e., guaranteed, satisfying property **i)** of Section 1.1.1. In the right part of this figure, we give the corresponding effectivity index (recall that this is the ratio of the estimate over the error,

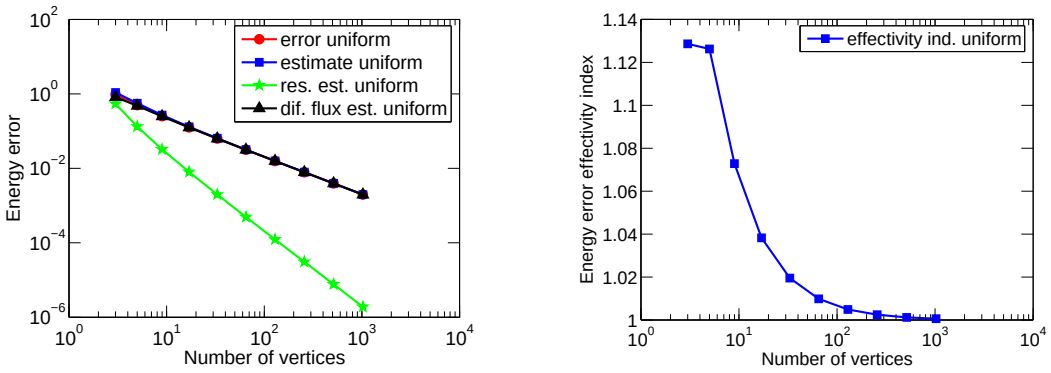

Figure 2.2: Estimated and actual energy error (left) and the corresponding effectivity index (right), vertex-centered finite volume method, problem (2.1a)–(2.1b) with a smooth solution in one space dimension

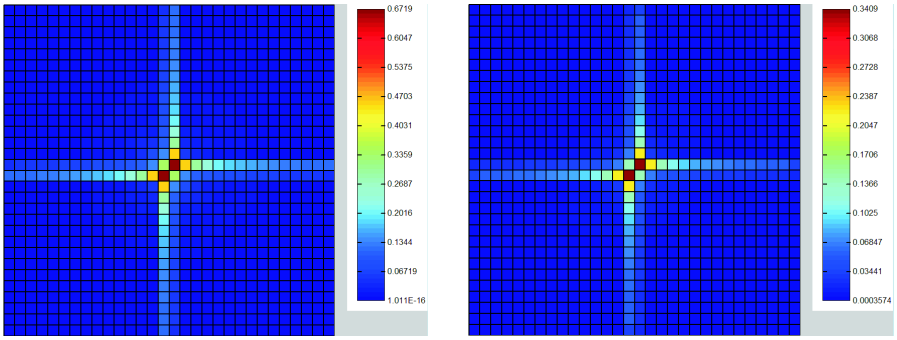

Figure 2.3: Estimated (left) and actual (right) energy error distribution, harmonic-weighted vertex-centered finite volume method, interface problem (2.1a)–(2.1b) with contrast 5 in the diffusion coefficient

bigger or equal to one as the estimate is guaranteed). In this particular case, we get the asymptotic exactness, property **iii)**.

As a second example, we present some results for a discontinuous diffusion coefficient with a checkerboard pattern distribution of [A13, Section 7.1.2]. Figure 2.3, left, shows the energy error distribution predicted by our a posteriori error estimate, whereas in its right part, we give the exact distribution. The fact that they match very well is a numerical evidence of the local efficiency, property **ii)**. In Figure 2.4, we next plot the effectivity indices for two different contrasts in the coefficients: 5 and 100. The fact that the two plots show similar values (close to one) is the numerical evidence of robustness, property **iv)**. Note finally that our estimates satisfy property **v)** of Section 1.1.1 as well, as, being evaluated on local patches, their evaluation cost is small.

For more computational examples, we refer to [A3] and [A13].

A unified framework for the error in the potentials

The estimate of Theorem 2.2.1 is only stated for the lowest-order finite element method (2.3). It, however, turns out that it holds in the same form for an arbitrary function $p_h \in H_0^1(\Omega)$, see its proof. We still need a more general result, as many numerical methods produce an approximation p_h such that it is from the space $H^1(K)$ for every mesh element $K \in \mathcal{T}_h$ but

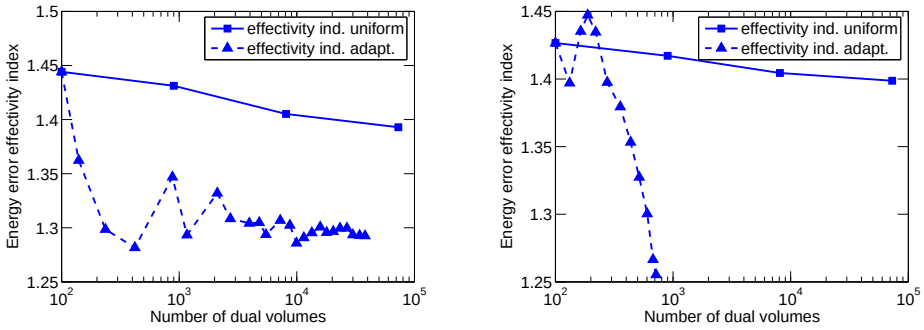

Figure 2.4: Energy error effectivity indices, harmonic-weighted vertex-centered finite volume method, interface problem (2.1a)–(2.1b) with contrast 5 (left) and 100 (right) in the diffusion coefficient

not from the space $H^1_0(\Omega)$ (we denote this space by $H^1(\mathcal{T}_h)$).

We have presented such a result in the preprint [84] (which is a part of Stephansen [148]) and in [A6] (in a more general convection–diffusion–reaction setting, see Section 2.2.6 below), cf. also [C1] and [C2]. We refer to [68, 6, 104, 69, 83, 116, 11] for closely related results. For some previous results, we refer to [72, 74, 2, 103, 34, 4].

In order to present this general result, we will need the following assumption:

Assumption 2.2.6 (Flux reconstruction for the diffusion problem (2.1a)–(2.1b))**.** *There exists a mesh $\mathcal{D}_h^*$, $\mathcal{D}_h^* = \mathcal{D}_h^{\mathrm{int},*} \cup \mathcal{D}_h^{\mathrm{ext},*}$, where the volumes in $\mathcal{D}_h^{\mathrm{ext},*}$ have a side lying in $\partial\Omega$, and there exists a vector field $\mathbf{t}_h \in \mathbf{H}(\mathrm{div},\Omega)$, arbitrary but such that*

$$(\nabla\cdot\mathbf{t}_h, 1)_D = (f,1)_D \qquad \forall D \in \mathcal{D}_h^{\mathrm{int},*}.$$

We then have (see [84, Theorem 3.7] and [A6, Theorem 3.1 and Lemma 4.1]):

Theorem 2.2.7 (Guaranteed estimates for the diffusion problem (2.1a)–(2.1b): a unified framework for the error in the potentials)**.** *Let p be the solution of (2.2) and let $p_h \in H^1(\mathcal{T}_h)$ be arbitrary. Let Assumption 2.2.6 be satisfied. Let finally $s_h \in H^1_0(\Omega)$ be arbitrary. Then*

$$|||p - p_h||| \le \left\{\sum_{D\in\mathcal{D}_h^*} \eta_{\mathrm{NC},D}^2\right\}^{\frac12} + \left\{\sum_{D\in\mathcal{D}_h^*} (\eta_{\mathrm{R},D} + \eta_{\mathrm{DF},D})^2\right\}^{\frac12},$$

where the nonconformity estimator *is given by*

$$\eta_{\mathrm{NC},D} := \|\mathbf{S}^{\frac12}\nabla(p_h - s_h)\|_D \qquad D \in \mathcal{D}_h^*, \tag{2.13}$$

the diffusive flux estimator $\eta_{\mathrm{DF},D}$ *is given by* (2.6)*, and the* residual estimator $\eta_{\mathrm{R},D}$ *is given by* (2.7)*.*

Remark that Theorem 2.2.7 has the same structure as Theorem 2.2.1, with, additionally, the estimators $\eta_{\mathrm{NC},D}$ stemming from the nonconformity of p_h, i.e., from the fact that $p_h \notin H^1_0(\Omega)$. The proof uses the same idea as that of Theorem 2.2.1, with, additionally, a triangle-like inequality for the treatment of the nonconformity, see [A11, Lemma 7.1]. Note also that the mesh $\mathcal{D}_h^*$ in Assumption 2.2.6 is very general and can be nonmatching and contain nonconvex or non-star-shaped elements. Typically, this mesh is either the original simplicial mesh $\mathcal{T}_h$, a dual mesh $\mathcal{D}_h$, or the fine simplicial mesh $\mathcal{S}_h$ of the previous section.

Remark 2.2.8 (Potential and flux reconstructions)**.** *Recall that the exact potential p is such that $p \in H^1_0(\Omega)$ and that the exact flux $-\mathbf{S}\nabla p$ is such that $-\mathbf{S}\nabla p \in \mathbf{H}(\mathrm{div},\Omega)$. In the setting of Theorem 2.2.7, the approximate solution p_h can be such that $p_h \notin H^1_0(\Omega)$ and the approximate flux $-\mathbf{S}\nabla p_h$ can be such that $-\mathbf{S}\nabla p_h \notin \mathbf{H}(\mathrm{div},\Omega)$. The functions s_h and $\mathbf{t}_h$ of Theorem 2.2.7, clearly stemming from the nonconformity of p_h and $-\mathbf{S}\nabla p_h$, are herein called respectively the* potential *and* flux reconstructions*.*

2.2.2 Pure diffusion equation: a unified framework for locally conservative methods

Many numerical methods, like the mixed finite element one, cf. Brezzi and Fortin [47] or Roberts and Thomas [143], the finite volume one, cf. Eymard et al. [88], mimetic finite difference, cf. Brezzi et al. [48], covolume, cf. Chou et al. [66] and other, directly (or almost directly) produce an approximation of the flux $\mathbf{u} := -\mathbf{S}\nabla p$. Then a natural problem one may pose is how to derive a posteriori error estimates for the error between an approximate flux $\mathbf{u}_h$ and the exact one $\mathbf{u}$, say, in the energy norm

$$|||\mathbf{u} - \mathbf{u}_h|||_* := \|\mathbf{S}^{-\frac{1}{2}}(\mathbf{u} - \mathbf{u}_h)\|. \tag{2.14}$$

I have investigated this problem in [A11, A14]. In particular, I have shown the following result (see [A14, Theorems 6.1 and 6.8]) (as these methods are typically locally conservative on the given (simplicial) mesh $\mathcal{T}_h$, there is no need here for a construction of a dual grid $\mathcal{D}_h$ or of the grid $\mathcal{S}_h$ as in the previous section):

Theorem 2.2.9 (Guaranteed estimates for the diffusion problem (2.1a)–(2.1b): a unified framework for the error in the fluxes)**.** *Let p be the solution of (2.2), let $\mathbf{u} := -\mathbf{S}\nabla p$, and let $\mathbf{u}_h \in \mathbf{H}(\mathrm{div},\Omega)$ be arbitrary but such that*

$$(\nabla\cdot\mathbf{u}_h, 1)_K = (f, 1)_K \qquad \forall K \in \mathcal{T}_h. \tag{2.15}$$

Let $s_h \in H^1_0(\Omega)$ be arbitrary. Then

$$|||\mathbf{u} - \mathbf{u}_h|||_* \le \left\{ \sum_{K\in\mathcal{T}_h} \left(\eta^2_{\mathrm{P},K} + \eta^2_{\mathrm{R},K}\right) \right\}^{\frac{1}{2}},$$

where the potential estimator *is given by*

$$\eta_{\mathrm{P},K} := |||\mathbf{u}_h + \mathbf{S}\nabla s_h|||_{*,K} \qquad K \in \mathcal{T}_h \tag{2.16}$$

and the residual estimator *by*

$$\eta_{\mathrm{R},K} := m_{K,\mathbf{S}}\|f - \nabla\cdot\mathbf{u}_h\|_K \qquad K \in \mathcal{T}_h, \tag{2.17}$$

with the weighting coefficient

$$m_{K,\mathbf{S}} := C^{\frac{1}{2}}_{\mathrm{P},K}\frac{h_K}{c^{\frac{1}{2}}_{\mathbf{S},K}}.$$

Recall that estimates for the error in the potentials are given by Theorem 2.2.7; combining Theorems 2.2.7 and 2.2.9, estimates for errors in both the potentials and fluxes are obtained.

In order to apply Theorems 2.2.7 and 2.2.9 to a given numerical method, a way of constructing of the potential reconstruction s_h is crucial. I believe that a right way is to obtain

s_h in two steps. Firstly, for many numerical methods such as the finite volume or the mixed finite element one, a local postprocessing is applied so as to obtain an improved potential $\tilde{p}_h$. In the case of mixed finite elements, this is proposed in [A11, Section 4.1] for the lowest-order case: on each element $K \in \mathcal{T}_h$, we define $\tilde{p}_h$ by (supposing that $\mathbf{S}$ is piecewise constant)

$$-\mathbf{S}\nabla\tilde{p}_h|_K = \mathbf{u}_h|_K, \tag{2.18a}$$

$$\frac{(\tilde{p}_h, 1)_K}{|K|} = p_h|_K; \tag{2.18b}$$

here $\mathbf{u}_h$ and p_h are the mixed finite element flux and potential approximations, respectively. For higher-order cases, I follow Arnold and Brezzi [19] and Arbogast and Chen [13], see [A14, Section 4.4.2]. I apply similar ideas to the case of finite volumes, see [A12, Section 3.2], taking inspiration from Eymard et al. [89]. The potential postprocessed by (2.18a)–(2.18b) or a similar procedure is typically nonconforming, not contained in $H_0^1(\Omega)$ (except in one space dimension). Thus, a second step is to apply to $\tilde{p}_h$ an averaging operator, yielding $s_h \in H_0^1(\Omega)$. In fact, I typically apply the a posteriori estimates of Theorems 2.2.7 and 2.2.9 to $\tilde{p}_h$ and not to p_h.

The crucial property of the locally postprocessed potential $\tilde{p}_h$ in mixed finite elements is that its traces on the sides of $\mathcal{T}_h$ are continuous in mean, i.e., $\langle\tilde{p}_h|_K, 1\rangle_{\sigma_{K,L}} = \langle\tilde{p}_h|_L, 1\rangle_{\sigma_{K,L}}$ for all interior sides $\sigma_{K,L}$ shared by elements K and L. One can then show the following theorem (see [A14, Theorem 6.16]):

Theorem 2.2.10 (Local efficiency of the estimates for the diffusion problem (2.1a)–(2.1b))**.** *For all $K \in \mathcal{T}_h$, there holds*

$$\eta_{\mathrm{P},K} \le \eta_{\mathrm{DF},K} + \eta_{\mathrm{NC},K}, \tag{2.19a}$$

$$\eta_{\mathrm{DF},K} \le |||\mathbf{u} - \mathbf{u}_h|||_{*,K} + |||p - \tilde{p}_h|||_K, \tag{2.19b}$$

$$\eta_{\mathrm{NC},K} \le C C_{\mathbf{S},K}^{\frac{1}{2}} c_{\mathbf{S},\mathcal{T}_K}^{-\frac{1}{2}} |||p - \tilde{p}_h|||_{\mathcal{T}_K}, \tag{2.19c}$$

$$\eta_{\mathrm{R},K} \le C C_{\mathbf{S},K}^{\frac{1}{2}} c_{\mathbf{S},K}^{-\frac{1}{2}} |||\mathbf{u} - \mathbf{u}_h|||_{*,K}, \tag{2.19d}$$

where the constant C depends only on the space dimension d, the maximal polynomial degree of $\mathbf{u}_h$ and $\tilde{p}_h$, the maximal polynomial degree of f, and on the shape regularity parameter of the mesh $\mathcal{T}_h$. In (2.19), $c_{\mathbf{S},\mathcal{T}_K}$ is the smallest eigenvalue that $\mathbf{S}$ takes on a patch $\mathcal{T}_K$ of all elements sharing a node with $K \in \mathcal{T}_h$ and $C_{\mathbf{S},K}$ is the largest eigenvalue that $\mathbf{S}$ takes on the element K.

The key tools of this proof are the properties of the averaging operator proven in Achdou et al. [2], Karakashian and Pascal [103], and Burman and Ern [49], together with the techniques already mentioned for the proof of Theorem 2.2.3.

As a numerical example, we give in Figure 2.5 the estimated and actual error distribution for a cell-centered finite volume discretization of a diffusion problem with a discontinuous coefficient (of contrast 5) with a checkerboard pattern distribution of [A12, Section 6.1]. The approximate solution and the corresponding adaptively refined mesh (for contrast 100) are given in Figure 2.6.

2.2.3 Pure diffusion equation: multiscale, multinumerics, and mortar coupling

We show here a further extension of the results of the previous section, presented in [B3].

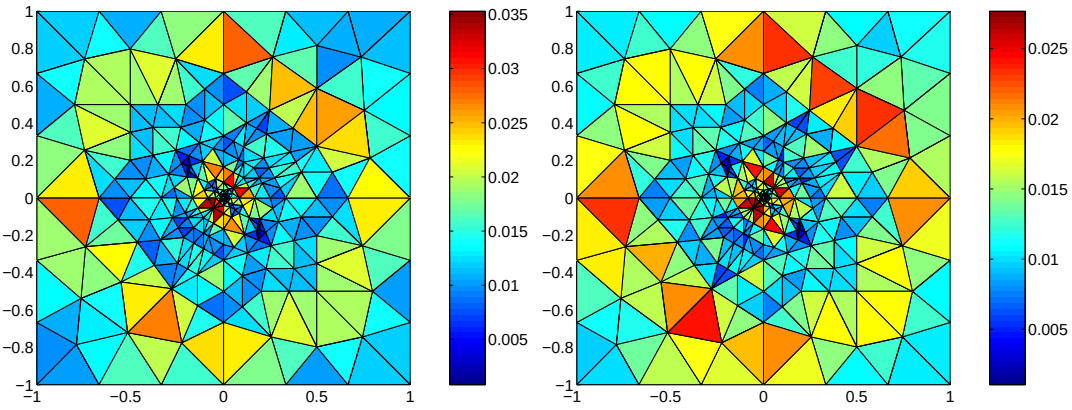

Figure 2.5: Estimated (left) and actual (right) energy error distribution, cell-centered finite volume method, interface problem (2.1a)–(2.1b) with contrast 5 in the diffusion coefficient

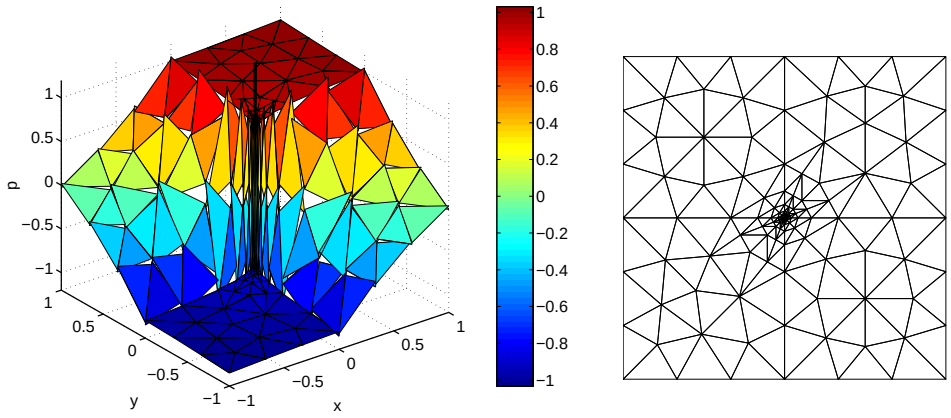

Figure 2.6: Approximate solution and the corresponding adaptively refined mesh, cell-centered finite volume method, interface problem (2.1a)–(2.1b) with contrast 100 in the diffusion coefficient

Firstly, we allow for a multinumerics setting, i.e., different numerical methods (mixed finite element, discontinuous Galerkin, finite volume) used in different parts of the domain. Secondly, the different subdomains can be meshed independently, resulting in a nonmatching grid. Thirdly, the mortar technique (cf. Bernardi et al. [40]) is supposed to be used in order to glue the approximations from the different subdomains. Lastly, the discretization can be done in the multiscale setting, allowing for the decomposition of the problem into h-scale subdomain problems and H-scale interface problems.

A unified framework for the error in the fluxes, as that of Theorem 2.2.9, is given in [B3, Theorems 3.2 and 3.3]. Similarly, a unified framework for the error in the potentials, as that of Theorem 2.2.7, is given in [B3, Theorems 3.4 and 3.5]. The potential reconstruction is carried along the lines described in Section 2.2.2. The flux reconstruction is more involved here, as it has to take into account the mortar error. Three different ways are proposed in Sections 3.3.2–3.3.4 of [B3]. The first one is based on a direct prescription, the second one the solution of h-grid-size low order local Neumann problems, and the last one on the solution of H-grid-size high order local Neumann problems. Local efficiency, in the spirit of Theorem 2.2.10, is also proven. Most importantly, this lower bound is robust with respect to the multiscale, i.e., robust

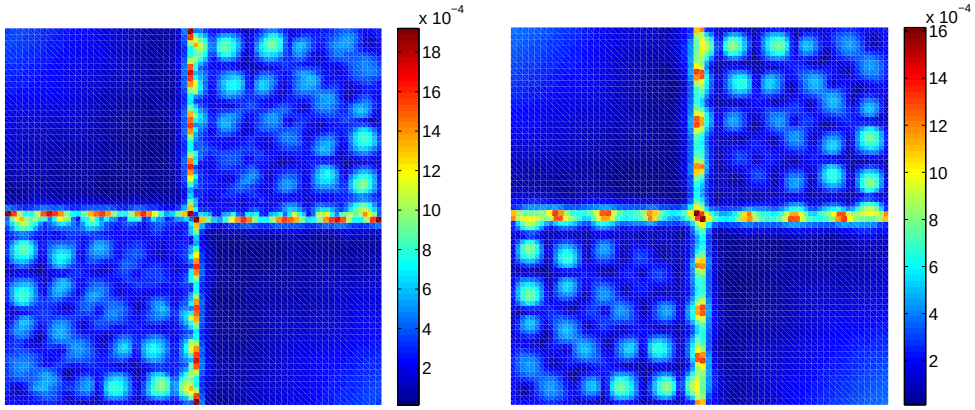

Figure 2.7: Estimated (left) and actual (right) flux error distribution on a nonmatching mesh with mortars, mortar mixed finite element method, problem (2.1a)–(2.1b)

with respect to the ratio H/h, for the last of the above three different flux reconstructions, see [B3, Theorems 4.2, 4.3, and 4.5]. There are two key steps for the lower bound proof. The first one is similar to that in the proof of Theorem 2.2.3 (analysis of local mixed finite element problems using local postprocessing). The second one is Lemma A.1 of [B3], an extension of the result of [2, Theorem 10] to the case of nonmatching grids.

Figure 2.7 gives a computational example for the mortar mixed finite element method of Arbogast et al. [14]. The interfaces along the x and y axes had nonmatching grids, coupled by the mortars. We can in particular see that our estimates predict well the error distribution not only inside the subdomains but also along the mortar interfaces. We refer to Section 3.3 below for an adaptive algorithm balancing the subdomain and mortar errors and another computational example (in the multinumerics setting).

2.2.4 Pure diffusion equation: taking into account the algebraic error

All the above results are presented under the assumption that the system of linear algebraic equations of the given numerical method applied to problem (2.1a)–(2.1b) has been solved exactly. Equivalently, this means that we need (2.5), Assumption 2.2.6, or (2.15) to hold exactly.

We have in [A10] derived a posteriori error estimates for the discretization of (2.1a)–(2.1b) by the cell-centered finite volume method which enable to take into account the algebraic error, i.e., allow for the algebraic system not to be solved exactly. More precisely, we suppose that instead of the solution algebraic vector P, which should satisfy

$$\mathbb{S}P = H$$

with $\mathbb{S}$ the finite volume system matrix and H the right-hand side, we only have P^{a} that satisfies

$$\mathbb{S}P^{\mathrm{a}} = H - R \tag{2.20}$$

for an algebraic residual vector R. Let f_K denote the mean value of the source term function f over $K \in \mathcal{T}_h$, $f_K := (f,1)_K/|K|$, let $\mathbf{RTN}(\mathcal{T}_h)$ stand for the lowest-order Raviart–Thomas–Nédélec space over the mesh $\mathcal{T}_h$, and recall the definition (2.4) of the energy error. The main result of [A10] can be presented in the following form (see Theorem 5.2 in this reference):

Theorem 2.2.11 (A posteriori error estimates for the diffusion problem (2.1a)–(2.1b) taking into account the algebraic error)**.** *Let p be the solution of (2.2). Let $\mathbf{u}_h^{\mathrm{a}}$ and p_h^{a} be the approximate flux and approximate potential, corresponding to (2.20). In particular, we suppose that $\mathbf{u}_h^{\mathrm{a}}$ is such that*

$$(\nabla\cdot\mathbf{u}_h^{\mathrm{a}},1)_K = (f,1)_K - R_K \qquad \forall K\in\mathcal{T}_h.$$

Let $\tilde{p}_h^{\mathrm{a}}$ be given by the local postprocessing on each $K\in\mathcal{T}_h$,

$$-\mathbf{S}\nabla\tilde{p}_h^{\mathrm{a}}|_K = \mathbf{u}_h^{\mathrm{a}}|_K,$$
$$\frac{(\tilde{p}_h^{\mathrm{a}},1)_K}{|K|} = p_h^{\mathrm{a}}|_K.$$

Let finally $s_h\in H_0^1(\Omega)$ be arbitrary. Then

$$|||p-\tilde{p}_h^{\mathrm{a}}||| \le \left\{\sum_{K\in\mathcal{T}_h}\eta_{\mathrm{NC},K}^2\right\}^{\frac12} + \left\{\sum_{K\in\mathcal{T}_h}\eta_{\mathrm{Osc},K}^2\right\}^{\frac12} + \eta_{\mathrm{AE}},$$

where the nonconformity estimator *is given by*

$$\eta_{\mathrm{NC},K} := \|\mathbf{S}^{\frac12}\nabla(\tilde{p}_h^{\mathrm{a}}-s_h)\|_K \qquad K\in\mathcal{T}_h,$$

the data oscillation estimator *is given by*

$$\eta_{\mathrm{Osc},K} := m_{K,\mathbf{S}}\|f-f_K\|_K \qquad K\in\mathcal{T}_h,$$

with the weighting coefficient

$$m_{K,\mathbf{S}} := C_{\mathrm{P},K}^{\frac12}\frac{h_K}{c_{\mathbf{S},K}^{\frac12}},$$

and the algebraic error estimator *is given by*

$$\eta_{\mathrm{AE}} := \inf_{\substack{\mathbf{r}_h\in\mathbf{RTN}(\mathcal{T}_h)\\ \nabla\cdot\mathbf{r}_h|_K=R_K/|K|}}\ \sup_{\substack{\varphi\in H_0^1(\Omega)\\ |||\varphi|||=1}} (\mathbf{r}_h,\nabla\varphi). \tag{2.22}$$

The algebraic error estimator η_{AE} of (2.22) is not (easily and locally) computable. Two easily, fully, and locally computable upper bounds on η_{AE} are derived in [A10]; η_{AE}^1 in Section 7.1 and η_{AE}^3 in Section 7.3. These two upper bounds are general as completely independent of the algebraic solver used; for the same reason, however, these upper bounds may overestimate the algebraic error. An approximation $\hat{\eta}_{\mathrm{AE}}^2$ of η_{AE}, tailored for the use of the conjugate gradient method, see Hestenes and Stiefel [98], as the algebraic solver, is also introduced in [A10, Section 7.2]. This approximation is extremely easy to compute and gives excellent computational results, even if it does not give an upper bound on η_{AE} (the overall a posteriori error estimate is not guaranteed in this last case).

Set

$$\eta_{\mathrm{NC}} := \left\{\sum_{K\in\mathcal{T}_h}\eta_{\mathrm{NC},K}^2\right\}^{\frac12}. \tag{2.23}$$

Under the condition that the algebraic error estimator η_{AE} (or its upper bound) is small in comparison with the nonconformity η_{NC} one, namely that

$$\eta_{\mathrm{AE}} \le \gamma\,\eta_{\mathrm{NC}}, \qquad 0<\gamma\le 1, \tag{2.24}$$

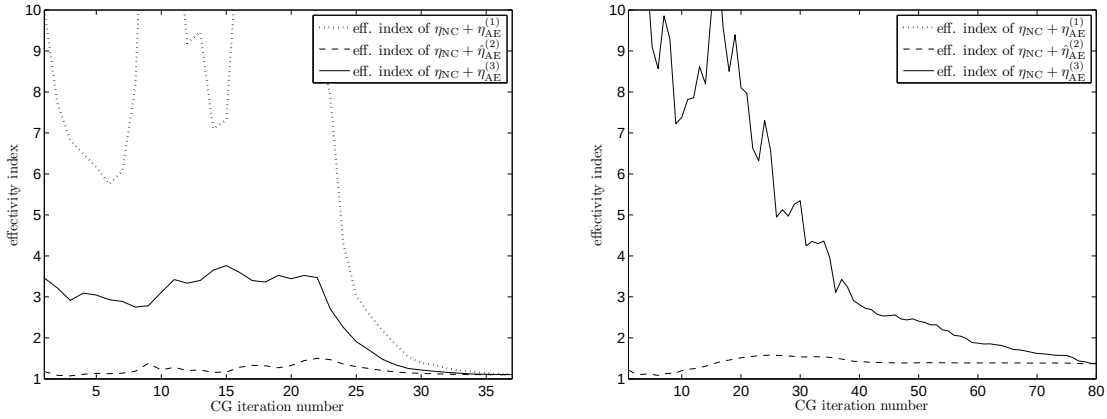

Figure 2.8: Effectivity indices for a posteriori error estimates including the algebraic error and the different algebraic estimators; problem (2.1a)–(2.1b) with a smooth solution (left) and with a contrast 100 in the diffusion coefficient (right)

for a parameter γ, typically chosen close to 1, we prove in [A10, Theorem 6.3] a global efficiency result of the form

$$\eta_{\mathrm{NC}} + \eta_{\mathrm{AE}} \leq C(1+\gamma)(|||p - \tilde{p}_h^{\mathrm{a}}||| + \text{ h.o.t.}), \tag{2.25}$$

where h.o.t. stands for higher-order terms and where the constant C depends only on the space dimension d, on the shape regularity parameter of the mesh $\mathcal{T}_h$, and on the local inhomogeneity and anisotropy ratio $\max_{K\in\mathcal{T}_h}\{C_{\mathbf{S},K}/c_{\mathbf{S},\mathcal{T}_K}\}$. Moreover, under the condition that the algebraic error estimator $\eta_{\mathrm{AE},K}$ is small in comparison with the nonconformity estimator $\eta_{\mathrm{NC},K}$ locally, element by element, namely that

$$\eta_{\mathrm{AE},K} \leq \gamma_K\, \eta_{\mathrm{NC},K}, \qquad 0 < \gamma_K \leq 1 \qquad \forall K \in \mathcal{T}_h, \tag{2.26}$$

for a set of parameters γ_K, typically chosen close to 1, we prove in [A10, Theorem 6.2] a local efficiency result of the form

$$\eta_{\mathrm{NC},K} + \eta_{\mathrm{AE},K} \leq (1+\gamma_K)(C C_{\mathbf{S},K}^{\frac{1}{2}} c_{\mathbf{S},\mathcal{T}_K}^{-\frac{1}{2}} |||p - \tilde{p}_h^{\mathrm{a}}|||_{\mathcal{T}_K} + \text{ h.o.t.}), \tag{2.27}$$

where the constant C depends only on the space dimension d and on the shape regularity parameter of the mesh $\mathcal{T}_h$. Note that (2.27) means that the a posteriori error estimate of Theorem 2.2.11 can be safely used for adaptive mesh refinement even in the presence of the algebraic error. Moreover, both (2.24) and (2.26) can be further used as a stopping criterion for iterative algebraic solvers, see Section 3.1 below.

The analysis of [A10] required in particular the coupling of the tools of numerical functional analysis and numerical linear algebra. Alternative variational formulations and elements of the duality theory were also necessary.

An example of a numerical result from [A10, Section 8] is presented in Figure 2.8. We consider there a fixed mesh and show the effectivity indices, i.e., the quantities $(\{\sum_{K\in\mathcal{T}_h}\eta_{\mathrm{NC},K}^2\}^{\frac{1}{2}} + \{\sum_{K\in\mathcal{T}_h}\eta_{\mathrm{Osc},K}^2\}^{\frac{1}{2}} + \eta_{\mathrm{AE}}^{\mathrm{approx}})/|||p-\tilde{p}_h^{\mathrm{a}}|||$, for the three above-mentioned computable approximations η_{AE}^1, $\hat{\eta}_{\mathrm{AE}}^2$, and η_{AE}^3 of η_{AE}, as a function of the number of iterations of the conjugate gradient method. Note in particular that the conjugate gradients-tailored estimator $\hat{\eta}_{\mathrm{AE}}^2$ of [A10, Section 7.2] gives effectivity indices systematically close to one from the very first iterations and thus controls optimally both the discretization and algebraic errors. More results are presented in Section 3.1 below.

2.2.5 Reaction–diffusion equation: guaranteed and robust estimates for conforming discretizations

The subject of the study in [A4] were a posteriori error estimates for the vertex-centered finite volume discretization of the problem

$$-\Delta p + rp = f \qquad \text{in } \Omega, \tag{2.28a}$$
$$p = 0 \qquad \text{on } \partial\Omega, \tag{2.28b}$$

where $r \in L^\infty(\Omega)$, $r \geq 0$, is a reaction coefficient and $f \in L^2(\Omega)$. Problem (2.28a)–(2.28b) is singularly perturbed in case of increased values of r.

In [A4], Theorems 3.1 and 3.2, we first give an extension of the characterization property (2.9) to problem (2.28a)–(2.28b). The first main result is the guaranteed upper bound of Theorem 4.4 of this reference, stating that

$$|||p - p_h||| \leq \left\{ \sum_{D \in \mathcal{D}_h} (\eta_{\mathrm{R},D} + \eta_{\mathrm{DF},D})^2 \right\}^{\frac{1}{2}},$$

where p is given by (2.28a)–(2.28b), p_h is the vertex-centered finite volume approximation,

$$|||p - p_h|||^2 := \|\nabla(p - p_h)\|^2 + \|r^{\frac{1}{2}}(p - p_h)\|^2$$

is the energy error, and $\eta_{\mathrm{R},D}$ and $\eta_{\mathrm{DF},D}$ are, respectively, the residual and diffusive flux estimators, fully computable quantities, adaptations of those of Theorem 2.2.1 to the reaction–diffusion case.

The second main result of [A4] is a robust lower bound of Theorem 5.1 of the form

$$\eta_{\mathrm{R},D} + \eta_{\mathrm{DF},D} \leq C|||p - p_h|||_D,$$

with a generic constant C as those of Theorem 2.2.3, independent of the size of the reaction function r. The tools are similar to those of Theorems 2.2.1 and 2.2.3, with the additional important results of [A4, Lemma 4.2], where Poincaré, Friedrichs, and trace inequalities-based (cf. Appendix A below) auxiliary estimates designed to cope optimally with the reaction dominance are derived. Finally, in [A4, Appendix], in continuation of [A3, Section 3], local discrete minimization problems in each dual volume $D \in \mathcal{D}_h$, designed to bring the value of the effectivity index down to one, independently of the reaction coefficient r, are derived.

Figure 2.9 gives the effectivity indices for a model problem of [A4, Section 6] in dependence on the reaction coefficient r ganging between 10^{-6} and 10^6. The original estimate (solid lines) and the local minimization estimate of [A4, Appendix] (dashed lines) are presented. We see that particularly the later one gives the effectivity index quite close to the optimal value of one, and this over the whole range of variation of r, which numerically confirms the robustness of our a posteriori error estimates. Overall, the properties **i)**, **ii)**, **iv)**, and **v)** of Section 1.1.1 are all satisfied completely and the property **iii)** is satisfied approximately.

2.2.6 Convection–diffusion–reaction equation: guaranteed (and robust) estimates for mixed finite element, finite volume, and discontinuous Galerkin discretizations

The papers [A11, A12] for mixed finite element and finite volume approximations, respectively, (and their advanced publication [C3]) were actually my first works on a posteriori error

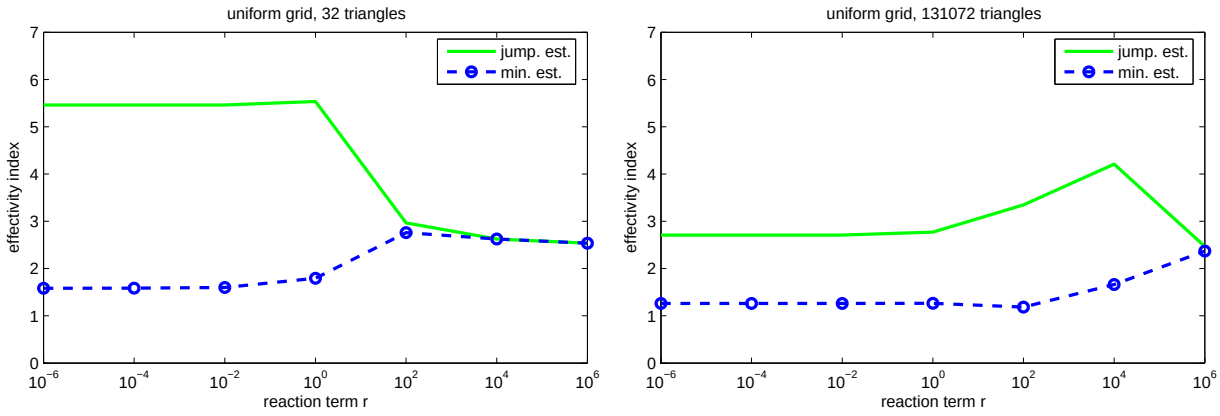

Figure 2.9: Effectivity indices in dependence on the reaction coefficient r of problem (2.28a)–(2.28b) for two different (uniformly refined) meshes, vertex-centered finite volume method

estimates. I consider therein the convection–diffusion–reaction equation

$$-\nabla\cdot(\mathbf{S}\nabla p) + \nabla\cdot(p\mathbf{w}) + rp = f \quad \text{in } \Omega, \tag{2.29a}$$

$$p = 0 \quad \text{on } \partial\Omega. \tag{2.29b}$$

General inhomogeneous Dirichlet and Neumann boundary conditions are treated in [A12] in place of (2.29b).

The estimates derived in [A11] take the form

$$|||p - \tilde{p}_h||| \le \left\{ \sum_{K\in\mathcal{T}_h} \eta_{\mathrm{NC},K}^2 \right\}^{\frac{1}{2}} + \left\{ \sum_{K\in\mathcal{T}_h} (\eta_{\mathrm{R},K} + \eta_{\mathrm{C},K} + \eta_{\mathrm{U},K})^2 \right\}^{\frac{1}{2}}, \tag{2.30}$$

where p is the weak solution of (2.29a)–(2.29b), $\tilde{p}_h$ is a local postprocessing of a mixed finite element approximation given by (2.18a)–(2.18b), and $\eta_{\mathrm{NC},K}$, $\eta_{\mathrm{R},K}$, $\eta_{\mathrm{C},K}$, and $\eta_{\mathrm{U},K}$ are respectively the nonconformity, residual, convection, and upwinding estimators, see [A11, Theorem 4.3]. The lower bound then writes, see [A11, Theorem 4.4]

$$\eta_{\mathrm{NC},K} + \eta_{\mathrm{R},K} + \eta_{\mathrm{C},K} \le |||p - \tilde{p}_h|||_{\mathcal{T}_K}(C_1 + C_2 \min\{\mathrm{Pe}_K, \varrho_K\}), \tag{2.31}$$

which implies overestimation by a factor proportional to the minimum of the local grid Péclet number Pe_K and the factor ϱ_K, defined by

$$\mathrm{Pe}_K := h_K \frac{C_{\mathbf{w},K}}{c_{\mathbf{S},K}}, \quad \varrho_K := \frac{C_{\mathbf{w},K}}{c_{\mathbf{w},r,K}^{\frac{1}{2}} c_{\mathbf{S},K}^{\frac{1}{2}}},$$

where $C_{\mathbf{w},K} = \|\mathbf{w}\|_{\infty,K}$ and $c_{\mathbf{w},r,K} = \frac{1}{2}\nabla\cdot\mathbf{w}|_K + r|_K$ (recall that $c_{\mathbf{S},K}$ is the smallest eigenvalue that $\mathbf{S}$ takes on K). Thus, the lower bound of (2.31) is not robust with respect to the convection dominance.

The missing robustness has been obtained in the collaboration [A6] in the discontinuous Galerkin setting, following an idea of Verfürth [168] (see also Schötzau and Zhu [146]). More precisely, the energy norm $|||v|||$ is replaced by the augmented norm

$$|||v|||_{\oplus} := |||v||| + \sup_{\varphi\in H_0^1(\Omega),\, |||\varphi|||=1} \{\mathcal{B}_{\mathrm{A}}(v,\varphi) + \mathcal{B}_{\mathrm{D}}(v,\varphi)\} \qquad v \in H^1(\mathcal{T}_h), \tag{2.32}$$

where $\mathcal{B}_{\mathrm{A}}$ is the skew-symmetric part of the differential operator associated with (2.29a) and where $\mathcal{B}_{\mathrm{D}}$, specific to the discontinuous Galerkin setting, is for all $u, v \in H^1(\mathcal{T}_h)$ defined by

$$\mathcal{B}_{\mathrm{D}}(u,v) := -\sum_{\sigma\in\mathcal{E}_h} \langle \mathbf{w}\cdot\mathbf{n}_\sigma [\![u]\!], \{\!\{\Pi_0 v\}\!\}\rangle_\sigma; \tag{2.33}$$

here $\mathcal{E}_h$ is the set of the sides of $\mathcal{T}_h$, $[\![\cdot]\!]$ is the operator denoting a jump across a side, and Π_0 stands for the L^2-orthogonal projection onto constants, see [A6, Section 3.2]. Still adding a jump seminorm contribution, $|||p-p_h|||_{\#,\mathcal{E}_h} = |||p_h|||_{\#,\mathcal{E}_h}$ (see [A6, equation (51)]), the final result, guaranteed upper bound which is fully robust in the singularly perturbed regimes resulting from dominant convection or reaction, can be written as

$$|||p-p_h|||_\oplus + |||p-p_h|||_{\#,\mathcal{E}_h} \le \widetilde{\eta} + |||p_h|||_{\#,\mathcal{E}_h} \le C(|||p-p_h|||_\oplus + |||p-p_h|||_{\#,\mathcal{E}_h}),$$

see [A6, Theorem 3.5]. Here p is the weak solution of (2.29a)–(2.29b), p_h is the discontinuous Galerkin approximation [A6, equations (14)–(15)], $\widetilde{\eta}$ and $|||p_h|||_{\#,\mathcal{E}_h}$ are fully computable estimators, and C is a generic constant in particular independent of the size of $\mathbf{w}$ and r.

Many additional analytical techniques and tools to those mentioned before have been used in [A6]. The upper bound, in the energy framework, is based on [A6, Lemma 4.1], a generalization of [A11, Lemma 7.1]. Its extension for the augmented norm (2.32) is given in [A6, Lemma 4.2]. The upper bound, as in Theorem 2.2.7, can be formulated quite generally. It relies on the notion of a potential reconstruction $s_h \in H^1_0(\Omega)$, a diffusive flux reconstruction $\mathbf{t}_h \in \mathbf{H}(\mathrm{div},\Omega)$, and a convective flux reconstruction $\mathbf{q}_h \in \mathbf{H}(\mathrm{div},\Omega)$. These reconstructions are supposed to satisfy, in a extension of Assumption 2.2.6,

$$(\nabla\cdot\mathbf{t}_h + \nabla\cdot\mathbf{q}_h + r p_h, 1)_K = (f,1)_K \qquad \forall K \in \mathcal{T}_h,$$

cf. [A6, equation (33)]. The way how to obtain the convective and diffusive flux reconstructions from the discontinuous Galerkin approximation is specified in [A6, equations (18)–(21)]. Treatment of the completely discontinuous functions is achieved via the specific jump seminorm, $|||\cdot|||_{\#,\mathcal{E}_h}$, see [A6, equation (51)]. Numerical experiments, see [A6, Section 5], confirm the robustness with respect to the convection dominance. Nonmatching meshes are also treated in [A6, Appendix].

2.2.7 The Stokes equation: a unified framework

The paper [B2] develops a unified framework for a posteriori error estimation for the Stokes problem, in continuation of the work in [A7].

We consider the Stokes problem in the form: given $\mathbf{f} \in [L^2(\Omega)]^d$, find $\mathbf{u}$, the velocity, and p, the pressure, such that

$$-\Delta\mathbf{u} + \nabla p = \mathbf{f} \quad \text{in} \quad \Omega, \tag{2.34a}$$
$$\nabla\cdot\mathbf{u} = 0 \quad \text{in} \quad \Omega, \tag{2.34b}$$
$$\mathbf{u} = \mathbf{0} \quad \text{on} \quad \partial\Omega. \tag{2.34c}$$

We suppose that the inf–sup condition holds with a positive constant β,

$$\inf_{q\in L^2_0(\Omega)} \sup_{\mathbf{v}\in[H^1_0(\Omega)]^d} \frac{(q,\nabla\cdot\mathbf{v})}{\|\nabla\mathbf{v}\|\,\|q\|} \ge \beta, \tag{2.35}$$

and define the energy (semi-)norm for $(\mathbf{v}, q) \in [H^1(\mathcal{T}_h)]^d \times L^2_0(\Omega)$ as

$$|||(\mathbf{v}, q)|||^2 := \|\nabla \mathbf{v}\|^2 + \beta^2 \|q\|^2. \tag{2.36}$$

Our estimates are based on the following assumption:

Assumption 2.2.12 (Flux reconstruction for the Stokes problem (2.34a)–(2.34c))**.** *There exists a tensor field* $\underline{\boldsymbol{\sigma}}_h \in \underline{\boldsymbol{H}}(\mathrm{div}, \Omega)$ *such that*

$$(\nabla \cdot \underline{\boldsymbol{\sigma}}_h + \mathbf{f}, \mathbf{e}_i)_K = 0, \quad i = 1, \dots, d, \quad \forall K \in \mathcal{T}_h, \tag{2.37}$$

where $\mathbf{e}_i \in \mathbb{R}^d$ *is the* i*-th Euclidean unit vector.*

We then have (see [B2, Theorem 5.1]):

Theorem 2.2.13 (Guaranteed estimates for the Stokes problem (2.34a)–(2.34c): a unified framework)**.** *Let* $(\mathbf{u}, p) \in [H^1_0(\Omega)]^d \times L^2_0(\Omega)$ *be the weak solution of* (2.34a)–(2.34c) *and let* $(\mathbf{u}_h, p_h) \in [H^1(\mathcal{T}_h)]^d \times L^2_0(\Omega)$ *be arbitrary. Choose an arbitrary* $\mathbf{s}_h \in [H^1_0(\Omega)]^d$ *and* $\underline{\boldsymbol{\sigma}}_h \in \underline{\boldsymbol{H}}(\mathrm{div}, \Omega)$ *which satisfies Assumption 2.2.12. Then it holds*

$$\begin{aligned} &|||(\mathbf{u} - \mathbf{u}_h, p - p_h)||| \\ &\le \left\{ \sum_{K \in \mathcal{T}_h} \eta^2_{\mathrm{NC},K} \right\}^{1/2} + \frac{1}{C_{\mathrm{S}}} \left\{ \sum_{K \in \mathcal{T}_h} \left\{ (\eta_{\mathrm{R},K} + \eta_{\mathrm{DF},K})^2 + \eta^2_{\mathrm{D},K} \right\} \right\}^{1/2}, \end{aligned}$$

where

$$\frac{1}{C_{\mathrm{S}}} \le \frac{2}{\sqrt{5} - 1}$$

and where the nonconformity estimator *is given by*

$$\eta_{\mathrm{NC},K} := \|\nabla(\mathbf{u}_h - \mathbf{s}_h)\|_K \qquad K \in \mathcal{T}_h,$$

the divergence estimator *is given by*

$$\eta_{\mathrm{D},K} := \frac{\|\nabla \cdot \mathbf{s}_h\|_K}{\beta} \qquad K \in \mathcal{T}_h,$$

the residual estimator *is given by*

$$\eta_{\mathrm{R},K} := C^{\frac{1}{2}}_{\mathrm{P},K} h_K \|\nabla \cdot \underline{\boldsymbol{\sigma}}_h + \mathbf{f}\|_K \qquad K \in \mathcal{T}_h,$$

and the diffusive flux estimator *is given by*

$$\eta_{\mathrm{DF},K} := \|\nabla \mathbf{s}_h - p_h \underline{\boldsymbol{I}} - \underline{\boldsymbol{\sigma}}_h\|_K \qquad K \in \mathcal{T}_h,$$

where $\underline{\boldsymbol{I}}$ *is a* $d \times d$ *identity matrix.*

A local lower bound is also derived in [B2, Theorem 6.1], under the following assumption:

Assumption 2.2.14 (Approximation property for the Stokes problem)**.** *For all* $K \in \mathcal{T}_h$*, there holds*

$$\|\nabla \mathbf{u}_h - p_h \underline{\boldsymbol{I}} - \underline{\boldsymbol{\sigma}}_h\|_K \le C \eta_{\mathrm{res},K}, \tag{2.38}$$

where C *is a generic constant and* $\eta_{\mathrm{res},K}$ *is the residual-based error indicator (see [B2, equation (6.1)]).*

Theorem 2.2.15 (Local efficiency for the Stokes problem (2.34a)–(2.34c))**.** *Let Assumption 2.2.14 hold. Then, for all $K \in \mathcal{T}_h$, there holds*

$$\eta_{\mathrm{NC},K} + \eta_{\mathrm{D},K} + \eta_{\mathrm{R},K} + \eta_{\mathrm{DF},K} \le C|||(\mathbf{u}-\mathbf{u}_h, p-p_h)|||_{\mathcal{T}_K} + C\left\{\sum_{\sigma\in\mathfrak{E}_K} h_\sigma^{-1}\|[\![\mathbf{u}_h]\!]\|_\sigma^2\right\}^{1/2}, \quad (2.39)$$

where C is a generic constant and $\mathfrak{E}_K$ stands for all the sides sharing a node with the element K (recall that $\mathcal{T}_K$ stands for all the elements sharing a node with the element K).

The ways how to construct on the discrete level the flux reconstruction $\underline{\boldsymbol{\sigma}}_h$ satisfying Assumptions 2.2.12 and 2.2.14 (and similar assumptions for the variants of [B2, Theorem 4.1 and Corollaries 5.1 and 5.2]) for different numerical methods, namely the various conforming and conforming stabilized finite element methods, the discontinuous Galerkin method, the Crouzeix–Raviart nonconforming finite element method, the mixed finite element method, and a general class of finite volume methods, are also given in [B2]. In particular, we extend in [B2, Section 7.2.2] to higher-order methods the approach of [A3, A13] and [C4] (see Section 2.2.1) through an equilibration technique in the spirit of Ainsworth and Oden [9], on the dual meshes $\mathcal{D}_h$. For conforming and conforming stabilized finite element methods, the last term of (2.39) vanishes, giving optimal local efficiency in the sense of property **ii)** of Section 1.1.1. In many other methods, it is also possible to bound this term by $|||(\mathbf{u}-\mathbf{u}_h, p-p_h)|||_{\mathcal{T}_K}$. In my opinion, the most important contribution of [B2] is that it gives a unified framework for a posteriori error estimates for the Stokes problem discretized by various numerical methods, optimal in the sense of the five optimal properties of Section 1.1.1 (up to exact asymptotic exactness). Supportive numerical experiments conclude [B2].

2.3 Stationary variational inequalities

I also had a chance to be involved in a collaboration on a posteriori error estimates for a system of variational inequalities, namely the contact between two membranes.

2.3.1 Contact between membranes: optimal estimates for conforming finite elements

The problem that we have studied in [A1] and [B1] writes: find p_1 and p_2, the displacements of two membranes, and λ, the action of the second membrane on the first one, verifying

$$-\mu_1\,\Delta p_1 - \lambda = f_1 \qquad \text{in } \Omega, \quad (2.40a)$$
$$-\mu_2\,\Delta p_2 + \lambda = f_2 \qquad \text{in } \Omega, \quad (2.40b)$$
$$p_1 - p_2 \ge 0, \quad \lambda \ge 0, \quad (p_1-p_2)\lambda = 0 \qquad \text{in } \Omega, \quad (2.40c)$$
$$p_1 = 0 \qquad \text{on } \partial\Omega, \quad (2.40d)$$
$$p_2 = 0 \qquad \text{on } \partial\Omega; \quad (2.40e)$$

here, μ_1 and μ_2 are positive constants representing the tensions of the membranes.

In [A1], we have derived residual a posteriori error estimates. These estimates do not satisfy property **i)** in the strict sense (an unknown generic constant appears) (see Theorem 7.2 and Corollary 7.3 in [A1]). Moreover, these estimates are not optimally locally efficient in the sense of property **ii)** (see Theorem 7.5 in [A1]). We have been able to improve these two properties in [B1]. Guaranteed and optimally locally efficient (up to a numerically negligible term) a

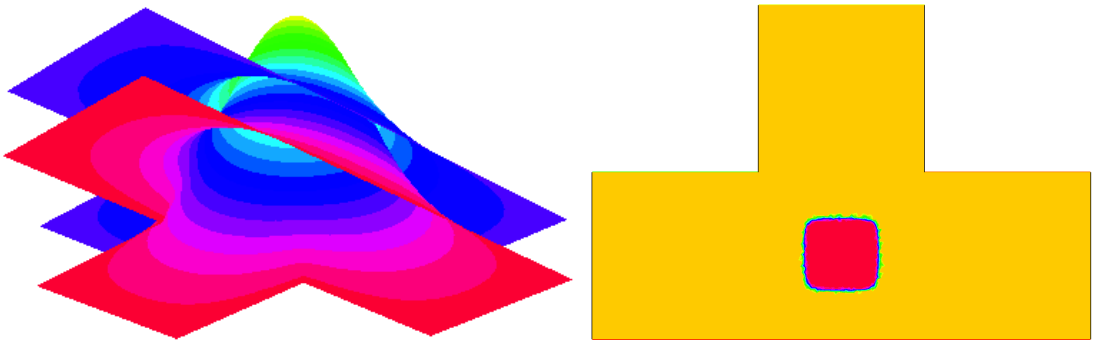

Figure 2.10: The displacements (left) and the action (right) for an adaptive discretization of the contact between membranes (2.40a)–(2.40e)

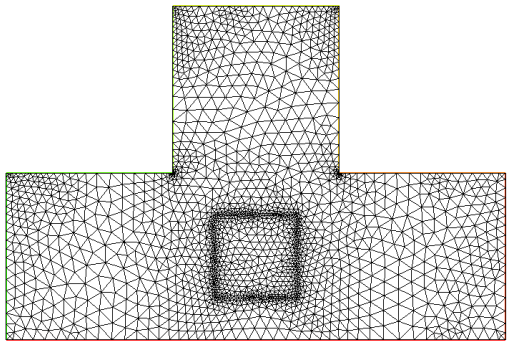

Figure 2.11: Adaptively refined mesh for the contact between membranes (2.40a)–(2.40e)

posteriori error estimates via a flux reconstruction similar to that described in Section 2.2.1 are derived in [B1], see Theorem 3.4 and Corollary 3.5 for the upper bound and Propositions 3.7–3.9 for the lower bound in this reference. To my best knowledge, such a result has not been obtained previously elsewhere.

Numerical experiments of [B1, Section 4] show the expected behavior. As an example, we show in Figure 2.10 the approximated displacements and the approximated action; Figure 2.11 then gives the corresponding adaptively refined mesh.

2.4 Stationary nonlinear problems

2.4.1 Monotone nonlinear problems: guaranteed and robust estimates for conforming finite elements

We have in [A5] considered the second-order monotone quasi-linear diffusion-type problem

$$-\nabla\cdot\boldsymbol{\sigma}(\nabla p) = f \quad \text{in } \Omega, \tag{2.41a}$$

$$p = 0 \quad \text{on } \partial\Omega, \tag{2.41b}$$

where the flux function $\boldsymbol{\sigma} : \mathbb{R}^d \to \mathbb{R}^d$ takes the quasi-linear form

$$\forall \boldsymbol{\xi} \in \mathbb{R}^d, \qquad \boldsymbol{\sigma}(\boldsymbol{\xi}) = a(|\boldsymbol{\xi}|)\boldsymbol{\xi}, \tag{2.42}$$

with $|\cdot|$ the Euclidean norm in $\mathbb{R}^d$ and $a : \mathbb{R}_+ \to \mathbb{R}$ a given function. The function a is assumed to satisfy a growth condition of the form $a(x) \sim x^{q-2}$ as $x \to +\infty$ for some real number

$q \in (1,+\infty)$, so that the natural energy space for the above model problem is the Sobolev space $W_0^{1,q}(\Omega)$. The problem (2.41a)–(2.41b) in weak form amounts to finding $p \in W_0^{1,q}(\Omega)$ such that

$$(\boldsymbol{\sigma}(\nabla p), \nabla v) = (f, v) \quad \forall v \in W_0^{1,q}(\Omega). \tag{2.43}$$

Let $p_{\mathrm{L},h}$ be an arbitrary function in $W_0^{1,q}(\Omega)$. The error measure used in [A5] is the dual norm of the residual,

$$\mathcal{J}_p(p_{\mathrm{L},h}) := \sup_{\varphi \in W_0^{1,q}(\Omega)\setminus\{0\}} \frac{(\boldsymbol{\sigma}(\nabla p) - \boldsymbol{\sigma}(\nabla p_{\mathrm{L},h}), \nabla\varphi)}{\|\nabla\varphi\|_q}. \tag{2.44}$$

Let r be the dual exponent of q, $r := q/(q-1)$. Similarly to Assumption 2.2.6, we will need below the following assumption:

Assumption 2.4.1 (Flux reconstruction for the nonlinear problem (2.41a)–(2.41b))**.** *There exists a mesh $\mathcal{D}_h^*$ and a vector field $\mathbf{t}_h \in \mathbf{W}^r(\mathrm{div},\Omega) := \{\mathbf{v} \in [L^r(\Omega)]^d;\ \nabla\cdot\mathbf{v} \in L^r(\Omega)\}$ such that*

$$(\nabla\cdot\mathbf{t}_h, 1)_D = (f,1)_D \qquad \forall D \in \mathcal{D}_h^{\mathrm{int},*}.$$

Let us introduce the linear or affine flux function $\boldsymbol{\sigma}_{\mathrm{L}} : \mathbb{R}^d \to \mathbb{R}^d$. This function is in practice obtained as, e.g., the Newton or the fixed point linearization of the function $\boldsymbol{\sigma}$ at a given function $p_0 \in W_0^{1,q}(\Omega)$. We then have, see [A5, Theorem 3.5], developing the ideas from Han [95] and Chaillou and Suri [61, 62]:

Theorem 2.4.2 (Guaranteed estimates for the monotone nonlinear problem (2.41a)–(2.41b))**.** *Let p be the solution of (2.43) and let $p_h \in W_0^{1,q}(\Omega)$ be arbitrary. Let Assumption 2.4.1 be satisfied. Then*

$$\mathcal{J}_p(p_{\mathrm{L},h}) \le \left\{\sum_{D\in\mathcal{D}_h^*} (\eta_{\mathrm{R},D} + \eta_{\mathrm{DF},D})^r\right\}^{\frac{1}{r}} + \left\{\sum_{D\in\mathcal{D}_h^*} \eta_{\mathrm{L},D}^r\right\}^{\frac{1}{r}},$$

where the diffusive flux estimator *is given by*

$$\eta_{\mathrm{DF},D} := \|\boldsymbol{\sigma}_{\mathrm{L}}(\nabla p_{\mathrm{L},h}) + \mathbf{t}_h\|_{r,D} \qquad D \in \mathcal{D}_h^*,$$

the residual estimator *is given by*

$$\eta_{\mathrm{R},D} := m_D \|f - \nabla\cdot\mathbf{t}_h\|_{r,D} \qquad D \in \mathcal{D}_h^*,$$

with the weighting coefficient m_D similar to that of (2.8), and the linearization estimator *is given by*

$$\eta_{\mathrm{L},D} := \|\boldsymbol{\sigma}(\nabla p_{\mathrm{L},h}) - \boldsymbol{\sigma}_{\mathrm{L}}(\nabla p_{\mathrm{L},h})\|_{r,D} \qquad D \in \mathcal{D}_h^*.$$

Set

$$\eta_{\mathrm{D}} := \left\{\sum_{D\in\mathcal{D}_h^*} (\eta_{\mathrm{R},D} + \eta_{\mathrm{DF},D})^r\right\}^{\frac{1}{r}} \tag{2.45}$$

the overall *discretization error estimator* and

$$\eta_{\mathrm{L}} := \left\{\sum_{D\in\mathcal{D}_h^*} \eta_{\mathrm{L},D}^r\right\}^{\frac{1}{r}} \tag{2.46}$$

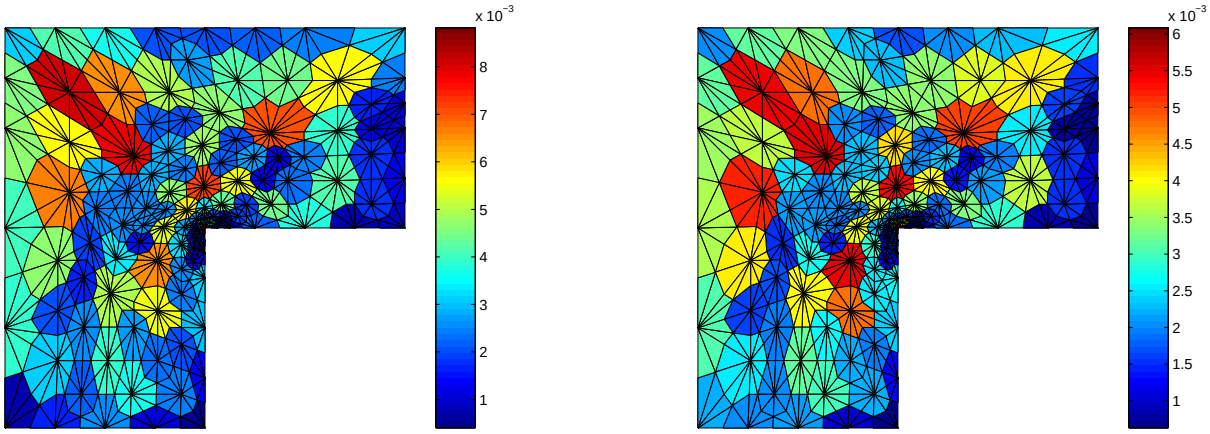

Figure 2.12: Estimated (left) and actual (right) error distribution; problem (2.41a)–(2.41b) with a singular solution, early stopped nonlinear solver

the overall linearization error estimator. Under the condition that the linearization error estimator η_{L} is small in comparison with the discretization η_{D} one, namely that

$$\eta_{\mathrm{L}} \leq \gamma\, \eta_{\mathrm{D}}, \qquad 0 < \gamma \leq 1, \tag{2.47}$$

for a parameter γ, typically chosen close to 1, we prove in [A5, Theorem 4.8] a global efficiency result of the form

$$\eta_{\mathrm{L}} + \eta_{\mathrm{D}} \leq C \mathcal{J}_p(p_{\mathrm{L},h}), \tag{2.48}$$

with a generic constant C in particular independent of the nonlinear function $\boldsymbol{\sigma}$. This means that our estimates are robust. I am not aware of another result which would give guaranteed and robust a posteriori error estimates for monotone nonlinear problems. Moreover, under the condition that the linearization error estimator $\eta_{\mathrm{L},D}$ is small in comparison with the discretization one $\eta_{\mathrm{R},D} + \eta_{\mathrm{DF},D}$ locally, dual volume by dual volume, namely that

$$\eta_{\mathrm{L},D} \leq \gamma_D\, (\eta_{\mathrm{R},D} + \eta_{\mathrm{DF},D}), \qquad 0 < \gamma_D \leq 1 \qquad \forall D \in \mathcal{D}_h^*, \tag{2.49}$$

for a set of parameters γ_D, typically chosen close to 1, we prove in [A5, Theorem 4.4] a local efficiency result of the form

$$\eta_{\mathrm{L},D} + \eta_{\mathrm{R},D} + \eta_{\mathrm{DF},D} \leq C \|\boldsymbol{\sigma}(\nabla p) - \boldsymbol{\sigma}(\nabla p_{\mathrm{L},h})\|_{r,D}, \tag{2.50}$$

with once again a generic constant C, independent of the nonlinear function $\boldsymbol{\sigma}$. Note that (2.50) means that the a posteriori error estimate of Theorem 2.4.2 can be safely used for adaptive mesh refinement even in the presence of the linearization error. Moreover, both (2.47) and (2.49) can be further used as a stopping criterion for iterative nonlinear solvers, such as the Newton or fixed-point ones, see Section 3.2 below.

An example of a numerical result from [A5, Section 6] is presented in Figure 2.12. We show there a predicted and actual error distribution for a case of a singular solution, obtained when the Newton method did not converge completely (the local stopping criterion (2.49) with $\gamma_D = 0.1$ was used). We see that even in this case, the predicted error distribution is excellent.

Many additional analytical techniques and tools to those mentioned before have been used in [A5]. The analysis relies on the notion of dual norms as $\mathcal{J}_p(p_{\mathrm{L},h})$ of (2.44), the ways how

to bound them from above and from below, and duality arguments. We work with Sobolev spaces $W_0^{1,q}(\Omega)$, in the L^q / L^r setting, and derive Lebesgue exponent q-robust inverse, bubble, Poincaré, and Friedrichs inequalities. Linearization techniques (e.g., Newton or fixed-point ones) are needed.

2.5 Instationary linear problems

I present here the contributions I had a chance to participate at concerning a posteriori error estimates for instationary linear problems.

2.5.1 The heat equation: a unified framework

In [A7], we have considered the heat equation

$$\partial_t p - \Delta p = f \quad \text{a.e. in } \Omega\times(0,T), \tag{2.51a}$$
$$p = 0 \quad \text{a.e. on } \partial\Omega\times(0,T), \tag{2.51b}$$
$$p(\cdot,0) = p_0 \quad \text{a.e. in } \Omega, \tag{2.51c}$$

with the final simulation time $T>0$, the source term $f\in L^2(\Omega\times(0,T))$, and the initial condition $p_0\in L^2(\Omega)$. The exact solution is such that $p\in X := L^2(0,T;H_0^1(\Omega))$ with $\partial_t p\in X' = L^2(0,T;H^{-1}(\Omega))$. For a.e. $t\in(0,T)$, there holds

$$\langle\partial_t p,\varphi\rangle(t) + (\nabla p,\nabla\varphi)(t) = (f,\varphi)(t) \qquad \forall\varphi\in H_0^1(\Omega). \tag{2.52}$$

Prior to presenting the main results, I need to introduce some more notation. Let $y\in X$. The space-time energy norm is given by

$$\|y\|_X^2 := \int_0^T \|\nabla y\|^2(t)\,\mathrm{d}t. \tag{2.53}$$

We take up the approach introduced by Verfürth [165] and measure the error in a numerical approximation of (2.51a)–(2.51c) in the above energy norm augmented by a dual norm of the time derivative: for $y\in Y := \{y\in X;\partial_t y\in X'\}$, we set

$$\|y\|_Y := \|y\|_X + \|\partial_t y\|_{X'}, \qquad \|\partial_t y\|_{X'} := \left\{\int_0^T \|\partial_t y\|_{H^{-1}}^2(t)\,\mathrm{d}t\right\}^{1/2}. \tag{2.54}$$

We allow the spatial meshes to evolve in time; we denote, for all time levels t^n, $0\le n\le N$, the associated mesh by $\mathcal{T}_h^n$. We suppose that the approximate solution on t^n, denoted by $p_{h\tau}^n$, is such that $p_{h\tau}^n\in H^1(\mathcal{T}_h^n)$ and we let $p_{h\tau}$ be the space-time approximate solution, given by $p_{h\tau}^n$ at each discrete time t^n and piecewise affine and continuous in time. We denote the space of such functions by $P_\tau^1(H^1(\mathcal{T}_h))$. We also denote by $P_\tau^1(H_0^1(\Omega))$ the space of functions piecewise affine and continuous in time and $H_0^1(\Omega)$ in space and $P_\tau^0(\mathbf{H}(\mathrm{div},\Omega))$ the space of functions piecewise constant in time and $\mathbf{H}(\mathrm{div},\Omega)$ in space. Set $\tau^n := t^n - t^{n-1}$, I_n the time interval $(t^{n-1},t^n]$, and $\widetilde{f}^n := \frac{1}{\tau^n}\int_{I_n} f(\cdot,t)\,\mathrm{d}t$, the in-time mean value of the data f. Let finally $\mathcal{T}_h^{n,n+1}$ be a common refinement of the two consecutive meshes $\mathcal{T}_h^n$ and $\mathcal{T}_h^{n+1}$.

As before in Sections 2.2.1, 2.2.2, 2.2.3, and 2.2.7, we intend to give a unified framework. For this reason, we introduce the following assumption, a space-time variant of the Assumptions 2.2.6, 2.4.1, and 2.2.12:

Assumption 2.5.1 (Potential and flux reconstructions for the heat problem (2.51a)–(2.51c))**.** *There exist respectively scalar and vector space-time fields*

$$s_{h\tau} \in P_\tau^1(H_0^1(\Omega)), \qquad \mathbf{t}_{h\tau} \in P_\tau^0(\mathbf{H}(\mathrm{div},\Omega)), \tag{2.55}$$

such that, for all $0 \le n \le N$,

$$(s_{h\tau}^n, 1)_K = (p_{h\tau}^n, 1)_K \qquad \forall K \in \mathcal{T}_h^{n,n+1}, \tag{2.56}$$

and, for all $1 \le n \le N$,

$$(\widetilde{f}^n - \partial_t p_{h\tau}^n - \nabla\cdot\mathbf{t}_{h\tau}^n, 1)_K = 0 \qquad \forall K \in \mathcal{T}_h^n. \tag{2.57}$$

Remark 2.5.2 (Assumption 2.5.1)**.** *Note that Assumption 2.5.1 means that the* potential reconstruction $s_{h\tau}$ preserves the elementwise mean values *of* $p_{h\tau}$*, whereas the* flux reconstruction $\mathbf{t}_{h\tau}$ is locally conservative*.*

Under Assumption 2.5.1, we have, see [A7, Theorem 3.2]:

Theorem 2.5.3 (Guaranteed estimate for the heat problem (2.51a)–(2.51c): a unified framework)**.** *Let* p *be the solution of* (2.52) *and let* $p_{h\tau} \in P_\tau^1(H^1(\mathcal{T}_h))$ *be arbitrary. Let Assumption 2.5.1 be satisfied. Then*

$$\begin{aligned}\|p - p_{h\tau}\|_Y \le 3 &\left\{\sum_{n=1}^N \int_{I_n} \sum_{K\in\mathcal{T}_h^n} (\eta_{\mathrm{R},K}^n + \eta_{\mathrm{DF},K}^n(t))^2 \,\mathrm{d}t\right\}^{1/2} + \eta_{\mathrm{IC}} + 3\|f - \widetilde{f}\|_{X'} \\ &+ \left\{\sum_{n=1}^N \int_{I_n} \sum_{K\in\mathcal{T}_h^n} (\eta_{\mathrm{NC},1,K}^n)^2(t) \,\mathrm{d}t\right\}^{1/2} + \left\{\sum_{n=1}^N \tau^n \sum_{K\in\mathcal{T}_h^n} (\eta_{\mathrm{NC},2,K}^n)^2\right\}^{1/2},\end{aligned}$$

where, for all $1 \le n \le N$ *and* $K \in \mathcal{T}_h^n$*, the* residual estimator *and the* diffusive flux estimator *are respectively given as*

$$\begin{aligned}\eta_{\mathrm{R},K}^n &:= C_{\mathrm{P},K}^{\frac{1}{2}} h_K \|\widetilde{f}^n - \partial_t s_{h\tau}^n - \nabla\cdot\mathbf{t}_{h\tau}^n\|_K, \\ \eta_{\mathrm{DF},K}^n(t) &:= \|\nabla s_{h\tau}(t) + \mathbf{t}_{h\tau}^n\|_K, \quad t \in I_n,\end{aligned}$$

with $C_{\mathrm{P},K} := 1/\pi^2$ *the constant from the Poincaré inequality* (A.1)*, and where the* nonconformity estimators *are given by*

$$\begin{aligned}\eta_{\mathrm{NC},1,K}^n(t) &:= \|\nabla(s_{h\tau} - p_{h\tau})(t)\|_K, \quad t \in I_n, \\ \eta_{\mathrm{NC},2,K}^n &:= C_{\mathrm{P},K}^{\frac{1}{2}} h_K \|\partial_t(s_{h\tau} - p_{h\tau})^n\|_K.\end{aligned}$$

Finally, the initial condition estimator *is given by*

$$\eta_{\mathrm{IC}} := 2^{1/2}\|s_{h\tau}^0 - p_0\|.$$

Note in particular that the estimate of Theorem 2.5.3 gives a guaranteed upper bound on the error measured in the augmented norm (2.54), and this in a unified framework, not relying on any particular numerical method.

We next intend to distinguish the space and time contributions to the error. For this reason, we define, for all $1 \le n \le N$,

$$(\eta_{\mathrm{sp}}^n)^2 := \sum_{K\in\mathcal{T}_h^n} 3\left\{\tau^n(9(\eta_{\mathrm{R},K}^n + \eta_{\mathrm{DF},1,K}^n)^2 + (\eta_{\mathrm{NC},2,K}^n)^2) + \int_{I_n} (\eta_{\mathrm{NC},1,K}^n)^2(t)\,\mathrm{d}t\right\},$$
$$(\eta_{\mathrm{tm}}^n)^2 := \sum_{K\in\mathcal{T}_h^n} 3\tau^n \|\nabla(s_{h\tau}^n - s_{h\tau}^{n-1})\|_K^2,$$

where

$$\eta_{\mathrm{DF},1,K}^n := \|\nabla s_{h\tau}^n + \mathbf{t}_{h\tau}^n\|_K.$$

We then have, see [A7, Theorem 3.6]:

Theorem 2.5.4 (Guaranteed estimate distinguishing space and time errors)**.** *Under the assumptions of Theorem 2.5.3, there holds*

$$\|p - p_{h\tau}\|_Y \le \left\{\sum_{n=1}^N (\eta_{\mathrm{sp}}^n)^2\right\}^{1/2} + \left\{\sum_{n=1}^N (\eta_{\mathrm{tm}}^n)^2\right\}^{1/2} + \eta_{\mathrm{IC}} + 3\|f - \widetilde{f}\|_{X'}.$$

Using this splitting, a space-time adaptive time-marching algorithm is proposed in [A7, Section 3.3], see also Section 3.4 below in the context of the convection–diffusion–reaction equation. This algorithm develops the ideas of Picasso [133], Verfürth [165], or Bergam et al. [38] and is designed to make the calculation efficient through balancing the spatial error parts η_{sp}^n and the temporal error parts η_{tm}^n. Moreover, it allows to achieve a user-given precision. Thus, efficiency and error control in the sense of Section 1.1 can be obtained.

We now turn to the efficiency of the estimate of Theorem 2.5.3. Define, for a set $\mathcal{E} \subset \mathcal{E}_h^n$ of the sides and a function $v \in \mathcal{T}_h^n$, the jump seminorms

$$|[\![v]\!]|_{\pm\frac12,\mathcal{E}} := \left\{\sum_{\sigma\in\mathcal{E}} h_\sigma^{\pm1}\|[\![v]\!]\|_\sigma^2\right\}^{1/2},$$

where h_σ denotes the diameter of the side σ. In order to present a lower bound in the unified framework as well, we need the following assumption (cf. Assumption 2.2.14):

Assumption 2.5.5 (Approximation property for the heat problem (2.51a)–(2.51c))**.** *We assume that for all $1 \le n \le N$ and for all $K \in \mathcal{T}_h^n$,*

$$\|\nabla p_{h\tau}^n + \mathbf{t}_{h\tau}^n\|_K \le C\left\{\sum_{L\in\mathcal{T}_K} h_L^2\|\widetilde{f}^n - \partial_t p_{h\tau}^n + \Delta p_{h\tau}^n\|_L^2\right\}^{1/2} + |[\![\nabla p_{h\tau}^n\cdot\mathbf{n}]\!]|_{+\frac12,\mathfrak{E}_K^{\mathrm{int},n}} + |[\![p_{h\tau}^n]\!]|_{-\frac12,\mathfrak{E}_K^n},$$

with a generic constant C, see [A7, equation (3.17)] (here $\mathcal{T}_K$ are all the elements sharing a node with K, $\mathfrak{E}_K^n$ are all the sides sharing a node with K, and $\mathfrak{E}_K^{\mathrm{int},n}$ are all the sides sharing a node with K in the interior of Ω).

Define a jump seminorm contribution term

$$\mathcal{J}^n(p_{h\tau})^2 := \tau^n \sum_{K\in\mathcal{T}_h^{n-1}} |[\![p_{h\tau}^{n-1}]\!]|_{-\frac12,\mathfrak{E}_K^{n-1}}^2 + \tau^n \sum_{K\in\mathcal{T}_h^n} |[\![p_{h\tau}^n]\!]|_{-\frac12,\mathfrak{E}_K^n}^2$$

and a data oscillation term

$$(\mathcal{E}_f^n)^2 := \|f - \widetilde{f}\|^2_{X'(I_n)} + \tau^n \sum_{K\in\mathcal{T}_h^n} h_K^2 \|\widetilde{f}^n - \Pi_{V_h^n}\widetilde{f}^n\|_K^2,$$

where V_h^n is the discrete approximation space. We then have, see [A7, Theorem 3.9]:

Theorem 2.5.6 (Local efficiency for the heat problem (2.51a)–(2.51c))**.** *Let Assumption 2.5.5 hold, let $1 \le n \le N$, and let both the refinement and coarsening in time be not too abrupt. Then*

$$\eta_{\mathrm{sp}}^n + \eta_{\mathrm{tm}}^n \le C(\|p - p_{h\tau}\|_{Y(I_n)} + \mathcal{J}^n(p_{h\tau}) + \mathcal{E}_f^n), \tag{2.58}$$

where C is a generic constant, in particular independent of the final simulation time T.

The lower bound of Theorem 2.5.6 is local in time but only global in space. This result is not fully optimal, as we are not sure to predict well the distribution of the error in space, and, consequently, to refine adequately the space mesh (compare it with the optimal situation for stationary problems in Section 2.2). However, it is of the same type as that achieved in Verfürth [165], and, to my best knowledge, local-in-time and local-in-space a posteriori error estimates for instationary problems have not been presented in the literature yet. Please also note the occurrence of the term $\mathcal{J}^n(p_{h\tau})$ on the right-hand side of (2.58). This term vanishes for conforming methods (finite elements or vertex-centered finite volumes) and can be bounded by $\|p-p_{h\tau}\|_{Y(I_n)}$ for many other methods, see [A7, Remark 3.10], so that only the error term $\|p-p_{h\tau}\|_{Y(I_n)}$ and the usual data oscillation term $\mathcal{E}_f^n$ are present on the right-hand side of (2.58).

To apply the above estimates to a given numerical method, one needs to verify Assumption 2.5.1 for the upper bound of Theorem 2.5.3 and Assumption 2.5.5 for the lower bound of Theorem 2.5.6. We show how to do this for the discontinuous Galerkin, various finite volume, mixed finite element, and conforming and nonconforming finite element methods in [A7, Section 4 and Appendix].

Some additional analytical techniques and tools to those mentioned before have been used in [A7]. Firstly, the analysis relies on the notion of space-time dual norms as $\|\cdot\|_{X'}$, cf. (2.54), and the ways how to bound them from above and from below. The space bubbles and inverse inequalities are in the heart of the important averaging operator satisfying the property (2.56). The time bubbles technique of Verfürth [165] has been used in the lower bound proof.

2.5.2 Convection–diffusion–reaction equation: conforming discretizations

In [A9], we have extended the results of [A7] to the instationary convection–diffusion–reaction setting in the context of vertex-centered finite volume methods. In particular a guaranteed upper bound similar to that of Theorem 2.5.3 has been derived in [A9, Theorem 4.2]. We have also in [A9, Theorem 4.1] derived an estimate for the energy norm only. As in Theorem 2.5.4, [A9, Corollary 4.6] gives an upper bound distinguishing the space and time error contributions. A space-time adaptive time marching algorithm, designed to achieve a user-given precision as efficiently as possible, is presented [A9, Section 6], see Section 3.4 below for its description. A lower bound similar to that of Theorem 2.5.6 is given in [A9, Theorem 4.7]. In particular, following Verfürth [167], robustness with respect to the convection dominance is shown in the dual norm setting.

One of the features of the analysis of [A9] is that it takes into account mass lumping, upwind weighting for the convection term, and the use of nonmatching grids, which are all

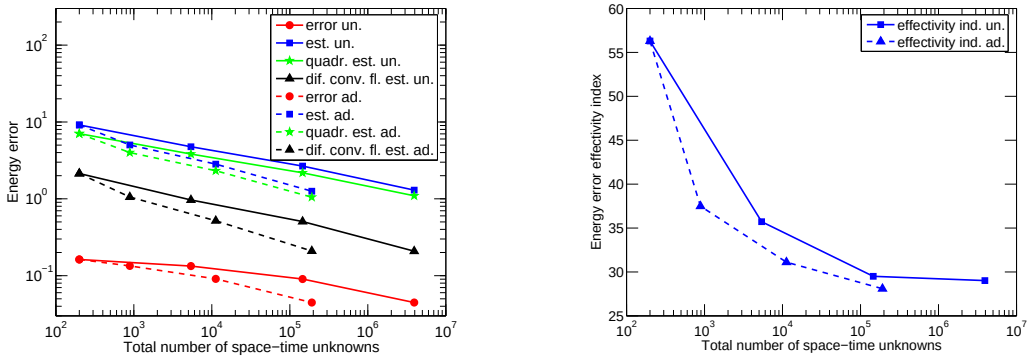

Figure 2.13: Estimated and actual energy error (left) and the corresponding effectivity index (right), combined finite volume–finite element method, instationary convection–diffusion–reaction problem

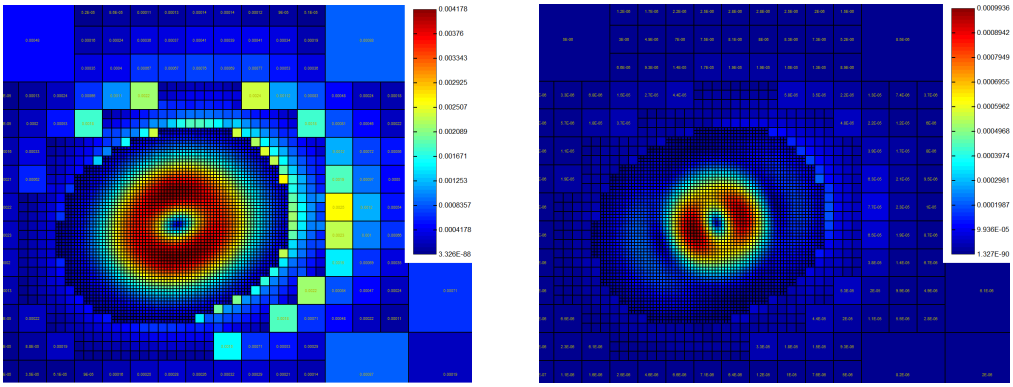

Figure 2.14: Estimated (left) and actual (right) energy error distribution, combined finite volume–finite element method, instationary convection–diffusion–reaction problem

useful and frequent in practice. The adaptive algorithm is implemented in the code TALISMAN [171] and numerical experiments are presented in [A9]. To give an example, we show in Figure 2.13 the estimated and actual energy error and the corresponding effectivity index for a model problem with a known solution. The results are similar to those of [A11, A12] in the stationary convection–diffusion–reaction setting: the effectivity index depends on the local grid Péclet number and only gets to optimal values once the local grid Péclet number gets small. Figure 2.14 then shows the predicted and actual error distribution. Although the theoretical result is, as in Theorem 2.5.6, global-in-space only, we can see from Figure 2.14 that the spatial error distribution is in practice predicted by our estimator reasonably well. Finally, in Figure 2.15, we present examples of approximate solutions. In particular, increasing the maximal refinement level (the right part in comparison with the left one) visibly helps to catch much better the steep exact solution. We refer for more examples to [A9, Section 7].

2.6 Instationary nonlinear problems

In the framework of the CNRS GNR MoMaS project *A posteriori estimates for efficient calculations and error control in numerical simulations of porous media* and also in the framework of the collaboration with the IFP, the French Petroleum Institute, via the ERT project *Enhanced*

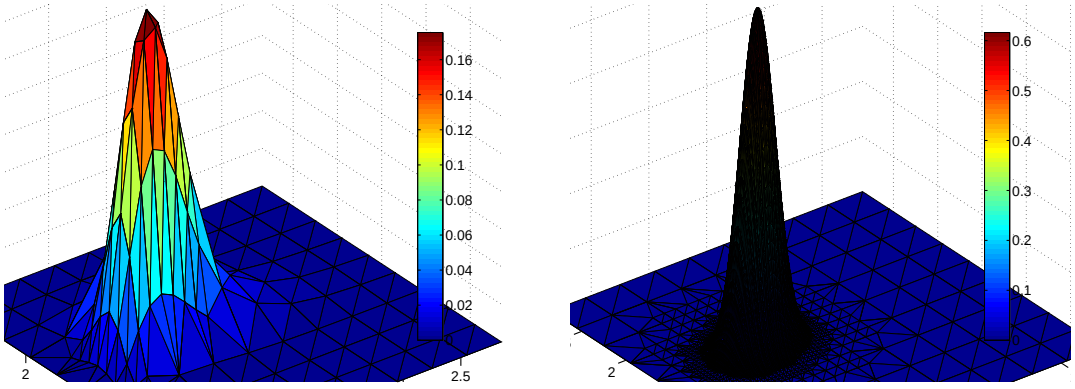

Figure 2.15: Examples of simulated plumes based on space-time adaptivity, two (left) and four (right) levels of refinement maximum, combined finite volume–finite element method, instationary convection–diffusion–reaction problem

oil recovery and geological sequestration of CO_2*: mesh adaptivity, a posteriori error control, and other advanced techniques*, I have recently been largely involved in instationary nonlinear problems. This topic represents a series of works in progress, with in particular three Ph.D. theses, see Section 5.2 below. The first results in this direction are those of [A10, A5, A7, A9], see Sections 2.2.4, 2.4.1, 2.5.1, and 2.5.2, respectively. As an example of an ongoing work, I give below some ideas for the two-phase flow.

2.6.1 Two-phase flow: guaranteed estimates

In [B4], I investigate the two-phase flow, given by the instationary nonlinear coupled system: find the phase saturations s_α, the phase pressures p_α, and the phase Darcy velocities $\mathbf{u}_\alpha$, $\alpha \in \{\mathrm{o}, \mathrm{w}\}$, such that

$$\partial_t(\phi s_\alpha) + \nabla\cdot\mathbf{u}_\alpha = q_\alpha \qquad \text{in } \Omega\times(0,T),\ \alpha\in\{\mathrm{o},\mathrm{w}\}, \tag{2.59a}$$

$$\mathbf{u}_\alpha = -\frac{k_{\mathrm{r},\alpha}(s_\mathrm{w})}{\mu_\alpha}\mathbf{K}(\nabla p_\alpha + \rho_\alpha g\nabla z) \qquad \text{in } \Omega\times(0,T),\ \alpha\in\{\mathrm{o},\mathrm{w}\}, \tag{2.59b}$$

$$s_\mathrm{o} + s_\mathrm{w} = 1 \qquad \text{in } \Omega\times(0,T), \tag{2.59c}$$

$$p_\mathrm{o} - p_\mathrm{w} = p_c(s_\mathrm{w}) \qquad \text{in } \Omega\times(0,T). \tag{2.59d}$$

The subscripts o, w stand for nonwetting and wetting phases, respectively. In the present context, the nonwetting phase is oil and the wetting one is water. In (2.59a)–(2.59d), the parameters which are only supposed to depend on the space coordinate $\mathbf{x}$ and the time t are the phase viscosities μ_α, the phase densities ρ_α, and the phase sources q_α, $\alpha\in\{\mathrm{o},\mathrm{w}\}$. For the sake of simplicity, I suppose that the porosity ϕ is constant in space and in time; $T>0$ is the final time. The system (2.59a)–(2.59d) is nonlinear and coupled because of the presence of p_c, the capillary pressure, and of $k_{\mathrm{r},\alpha}$, the phase relative permeabilities, which are both given functions of s_w. For the sake of simplicity of the mathematical analysis only, we suppose homogeneous Dirichlet boundary conditions

$$s_\mathrm{o} = 0 \qquad \text{on } \partial\Omega\times(0,T), \tag{2.60a}$$

$$p_\mathrm{w} = 0 \qquad \text{on } \partial\Omega\times(0,T). \tag{2.60b}$$

The initial condition is imposed through

$$s_\mathrm{o}(\cdot,0) = s_\mathrm{o}^0 \qquad \text{in } \Omega. \tag{2.61}$$

In continuation of the results presented in Sections 2.2.4, 2.4.1, and 2.5.1, I have first derived guaranteed a posteriori error estimates for the problem (2.59a)–(2.61), and this in a unified setting, independent of the particular numerical method. The main result of [B4] in this direction is the equivalent of Theorems 2.2.7, 2.2.11, 2.4.2, and 2.5.3, stating that

$$\begin{aligned}|||(s_\alpha - s_{\alpha,h\tau}, p_\alpha - p_{\alpha,h\tau})||| \leq &\left\{\sum_{n=1}^{N}\int_{I_n}\sum_{K\in\mathcal{T}_h^n}(\eta^n_{\mathrm{R},K,\alpha}+\eta^n_{\mathrm{DF},K,\alpha}(t))^2\,\mathrm{d}t\right\}^{\frac{1}{2}}\\ &+\left\{\sum_{n=1}^{N}\int_{I_n}\sum_{K\in\mathcal{T}_h^n}(\eta^n_{\mathrm{NC},K,\alpha}(t))^2\,\mathrm{d}t\right\}^{\frac{1}{2}}.\end{aligned} \tag{2.62}$$

Here $|||\cdot,\cdot|||$ stands for a dual norm similar to that of (2.44) and $\eta^n_{\mathrm{R},K,\alpha}$, $\eta^n_{\mathrm{DF},K,\alpha}$, and $\eta^n_{\mathrm{NC},K,\alpha}$ are fully computable estimators as those of Theorem 2.5.3.

In [B4], I have also distinguished, estimated separately, and compared the different error sources. This allows for efficient calculations through equilibration of the principal components and stopping criteria for the various involved iterative procedures. Section 3.5 below gives more details.

Chapter 3

Stopping criteria for linear and nonlinear iterative solvers and adaptive discretizations

The results presented in this short chapter are entirely based on the a posteriori error estimates of Chapter 2. I could have presented them directly in Chapter 2, but I prefer to do so here, so as to stress their, in my opinion, big importance. The motivation here is to achieve efficient calculation and error control in the sense of Section 1.1.

3.1 Stopping criteria for linear algebraic solvers

I have in Section 2.2.4 presented a posteriori error estimates of [A10], enabling to take into account the error stemming from the fact that an iterative algebraic solver did not converge completely. It turns out that the conditions (2.24) or (2.26) represent natural stopping criteria for linear algebraic solvers. Let us explain the major idea, see also Becker et al. [35], Patera and Rønquist [129], Arioli et al. [18], Arioli and Loghin [17], Picasso [134], and Silvester and Simoncini [147], on the example of Figure 3.1.

In this figure, we plot the evolution of the energy error as a function of the number of iterations of the conjugate gradients iterative solver for the model problem (2.1a)–(2.1b) discretized by the cell-centered finite volume method. The behavior is characteristic: in first cca 23 iterations, the error decreases, but it stagnates for all successive iterations. The reason for that is that the error has two components, the algebraic one, stemming from the fact that the system of linear equations is not solved exactly, and the discretization one, stemming from the mesh size and approximation properties of the finite volume solution. At the beginning (we start from a zero initial vector), the algebraic error dominates. Then, however, the algebraic error gets small in comparison with the discretization one, and the overall error stagnates, as the discretization error (which does not change with the iterations) becomes dominant. It shows that our nonconformity estimator η_{NC} (2.23) represents a reasonable approximation of the discretization error, see the behavior of η_{NC} in Figure 3.1. Similarly, the algebraic error estimator η^3_{AE} (recall that this is an upper bound on η_{AE} (2.22)) represents the algebraic error. Then our stopping criterion (2.24) roughly says that we should stop the algebraic solver iteration when the curves of η_{NC} and η^3_{AE} cross. The property (2.25) testifies that it is safe to do so. An important number of the algebraic solver iterations, where the overall error does not improve anymore and where the CPU time is literally wasted, may be sparred. In Figure 3.1, we also

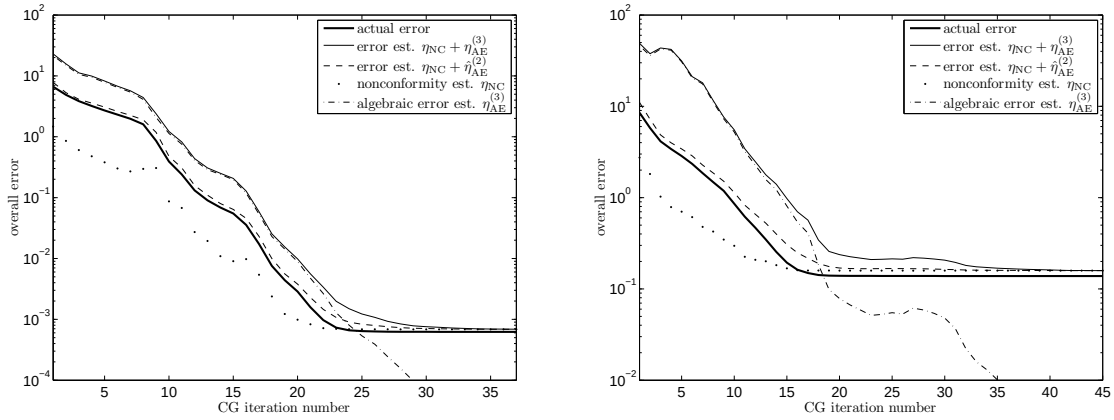

Figure 3.1: Energy error, overall estimators, and the algebraic and discretization estimators as a function of the number of iterations of the conjugate gradients iterative solver; problem (2.1a)–(2.1b) with a smooth solution (left) and with a contrast 100 in the diffusion coefficient (right)

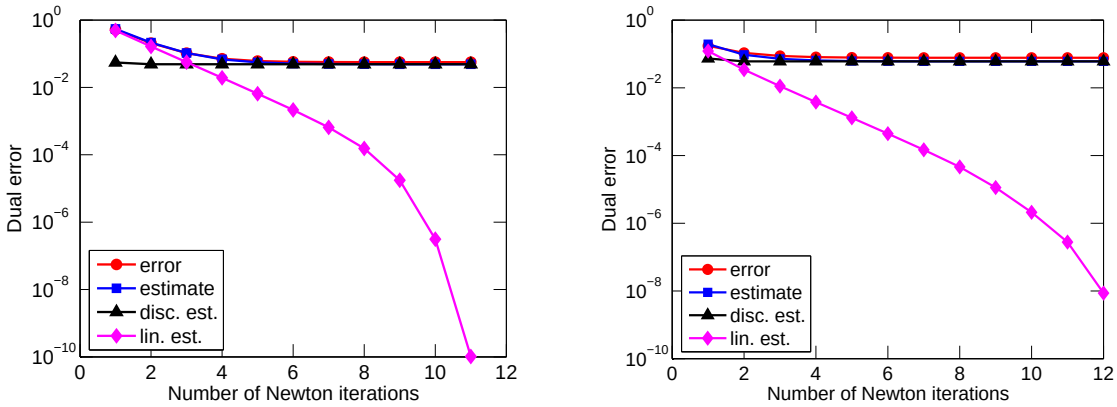

Figure 3.2: Dual error, overall estimator, and the linearization and discretization estimators as a function of the number of iterations of the Newton iterative solver; problem (2.41a)–(2.41b) with $q = 10$ (left) and $q = 50$ (right)

plot two overall estimators ($\eta_{NC}+\eta_{AE}^{3}$ and $\eta_{NC}+\hat{\eta}_{AE}^{2}$) (the data oscillation estimators $\eta_{Osc,K}$ are zero here) showing our final error estimate including the algebraic error (the corresponding effectivity indices were reported in Figure 2.8).

3.2 Stopping criteria for nonlinear solvers

I have in Section 2.4.1 presented a posteriori error estimates of [A5], enabling to take into account the error stemming from the fact that an iterative nonlinear solver did not converge completely. It turns out that the conditions (2.47) or (2.49) represent natural stopping criteria for nonlinear solvers, as in the previous section for linear solvers. The major idea is apparent from the example of Figure 3.2.

In this figure, we plot the evolution of the dual error as a function of the number of iterations of the Newton iterative nonlinear solver for the model problem (2.41a)–(2.41b) discretized by

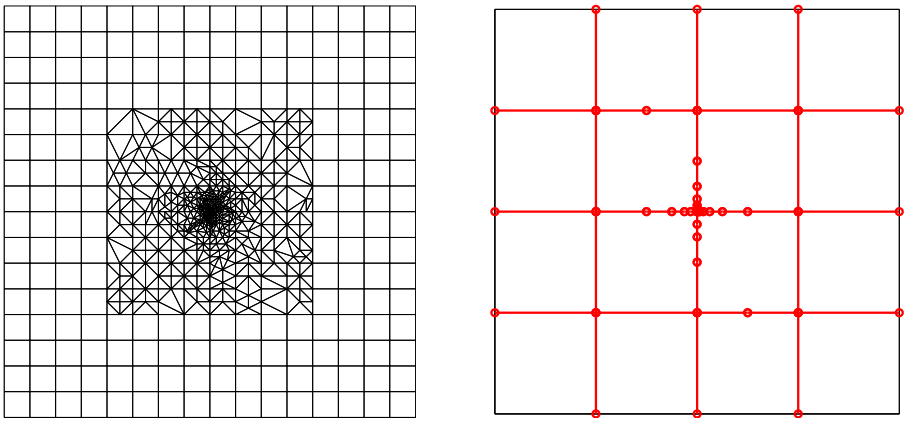

Figure 3.3: Adaptive subdomain (left) and mortar (right) meshes, mortar-coupled discontinuous Galerkin–mixed finite element method, problem (2.1a)–(2.1b)

the finite element method. The behavior is characteristic: in first cca 5 iterations, the error decreases, but it stagnates for all successive iterations. The reason for that is that the error has two components, the linearization one, stemming from the fact that the system of nonlinear equations is not solved exactly, and the discretization one, stemming from the mesh size and approximation properties of the finite element solution. At the beginning, the linearization error dominates. Then, however, the linearization error gets small in comparison with the discretization one, and the overall error stagnates, as the discretization error (which does not change with the iterations) becomes dominant. It shows that our discretization estimator η_{D} (2.45) represents a reasonable approximation of the discretization error, see its behavior in Figure 3.2. Similarly, the linearization error estimator η_{L} (2.46) represents the linearization error. Then our stopping criterion (2.47) roughly says that we should stop the linearization solver iteration when the curves of η_{D} and η_{L} cross. The property (2.48) testifies that it is safe to do so. An important number of the linearization solver iterations, where the overall error does not improve anymore and where the CPU time is literally wasted, may be sparred.

3.3 Balancing the subdomain and interface errors in mortar discretizations

In Section 2.2.3, we have derived a posteriori error estimates including the error from the use of mortars on the interfaces between subdomains. Our a posteriori error estimates, as in the case of Sections 3.1 and 3.2, enable to distinguish the different components of the error. In the present case, it is the subdomain discretization error, stemming from the mesh size and approximation properties of the given numerical method in the interiors of the subdomains, and the mortar discretization error, stemming from the use of mortars to glue the solution over the nonmatching interface. Following Wheeler and Yotov [175], and using the same detailed concepts as in Sections 3.1 and 3.2, an adaptive algorithm is designed to balance these two error components, see [B3, Section 8.3]. Figure 3.3 shows the performance of this algorithm. Remark that both the subdomain meshes and the mortar interface meshes are refined in the vicinity of the singularity residing in the origin.

Parameter	Meaning
N_{sp}	maximal level of space refinement
N_{tm}	maximal level of time refinement
`Ref`	percentage of cells for the space mesh refinement
`Deref`	percentage of cells for the space mesh derefinement
`Bulk`	spatial error estimate fraction for the derefinement
`DerefSp`	error estimate percentage for the space mesh derefinement
`DerefTm`	error estimate percentage for the time mesh derefinement
`Comp`	parameter for comparison of η_{sp} and η_{tm}
`StepsSpDeref`	number of steps after which the space mesh is derefined
`StepsTmDeref`	number of steps after which the time mesh is derefined

Table 3.1: Different parameters of the adaptive algorithm and their meaning

3.4 An adaptive discretization of an instationary convection–diffusion–reaction problem allowing to achieve a given precision

Building upon the ideas of Picasso [133], Verfürth [165], and Bergam et al. [38], space-time adaptive time-marching algorithms are proposed in [A7, Section 3.3] and [A9, Section 6]. The purpose is twofold. Firstly, we want that the algorithm automatically achieves a user-given relative precision, say ε, i.e., that

$$\frac{\sum_{n=1}^{N}(\eta_{\mathrm{sp}}^n+\eta_{\mathrm{tm}}^n)^2}{\sum_{n=1}^{N}\|p_{h\tau}\|^2_{X(t_{n-1},t_n)}}\leq\varepsilon^2. \tag{3.1}$$

Secondly, we want the calculation to be efficient. Using the fact that there are no unknown constants hidden in both η_{sp}^n and η_{tm}^n, we achieve this through balancing the spatial error parts η_{sp}^n and the temporal error parts η_{tm}^n. The algorithm is thus designed to, on each time level t_{n-1}, choose the space mesh $\mathcal{D}_h^n$ and time step τ_n such that

$$\eta_{\mathrm{sp}}^n\approx\varepsilon\frac{\|p_{h\tau}\|_{X(t_{n-1},t_n)}}{2},\quad \eta_{\mathrm{tm}}^n\approx\varepsilon\frac{\|p_{h\tau}\|_{X(t_{n-1},t_n)}}{2}.$$

For practical implementation purposes, we introduce the maximal refinement level parameters N_{sp} and N_{tm}. Some other parameters of the algorithm are listed in Table 3.1. We also denote by `SpTmUnkn` the total number of space–time unknowns. The actual algorithm is as follows:

- let an initial mesh $\mathcal{D}_h^0$ and an initial time step τ_1 be given
- set up the initial conditions on $\mathcal{D}_h^0$
- set $t_0=t_1=0$, $\mathcal{D}_h^1=\mathcal{D}_h^0$, and $n=1$
- set `EstSpPrev` $=1$, `EstTmPrev` $=0$
- set `LevTmRef` $=0$, `SpTmUnkn` $=0$
- set $\eta=0$

while $t_n<T$

- set `Count` $=0$

- set $t_n = t_{n-1} + \tau_n$
- set up the boundary conditions on $\mathcal{D}_h^n$
- set $\eta_{\mathrm{sp}}^n = \texttt{Crit} = 1$, $\texttt{ItSpRef} = 1$
- **while** $\eta_{\mathrm{sp}}^n \geq \texttt{Crit}$, $\texttt{ItSpRef} \leq N_{\mathrm{sp}} + 1$, and $\texttt{EstSpPrev} > \texttt{Comp} \cdot \texttt{EstTmPrev}$ when $\texttt{ItSpRef} \neq 1$
  - **if** $\texttt{ItSpRef} > 1$
    - refine such cells $D \in \mathcal{D}_h^n$ where $\eta_{D,\mathrm{sp}}^n \geq \texttt{Ref} \cdot \max_{E \in \mathcal{D}_h^n} \eta_{E,\mathrm{sp}}^n$ and such that their level of refinement is less than N_{sp}
    - create a new mesh $\mathcal{D}_h^n$ and interpolate the data onto this new mesh
  - solve the discrete problem on $\mathcal{D}_h^n$ with the time step τ_n to get new $p_{h\tau}|_{[t_{n-1},t_n]}$
  - compute the space a posteriori error estimate η_{sp}^n
  - set $\texttt{EstSpPrev} = \eta_{\mathrm{sp}}^n / \sqrt{\tau}_n$
  - compute the norm of the approximate solution $\|p_{h\tau}\|_{X(t_{n-1},t_n)}$ and set $\texttt{Crit} = \varepsilon \cdot \|p_{h\tau}\|_{X(t_{n-1},t_n)}/2$
  - set $\texttt{ItSpRef} = \texttt{ItSpRef} + 1$
- compute the time a posteriori error estimate η_{tm}^n
- set $\texttt{EstTmPrev} = \eta_{\mathrm{tm}}^n / \sqrt{\tau}_n$
- **if** $\eta_{\mathrm{tm}}^n \geq \texttt{Crit}$, $\texttt{LevTmRef} < N_{\mathrm{tm}}$, and $\texttt{EstTmPrev} > \texttt{Comp} \cdot \texttt{EstSpPrev}$
  - set $t_n = t_n - \tau_n$, $\tau_n = \tau_n/3$, and $\texttt{LevTmRef} = \texttt{LevTmRef} + 1$
- **else**
  - $\eta^2 = \eta^2 + \left(\eta_{\mathrm{tm}}^n + \eta_{\mathrm{sp}}^n\right)^2$
  - $\texttt{SpTmUnkn} = \texttt{SpTmUnkn} + |\mathcal{D}_h^n|$
  - $\texttt{Count} = \texttt{Count} + 1$
  - **if** $\texttt{Count}$ is a multiple of $\texttt{StepsSpDeref}$
    - set $\texttt{NBulkCells}$ as the number of cells which contain $\texttt{Bulk} \cdot \texttt{EstSpPrev}$ part of the spatial error
    - derefine such cells $D \in \mathcal{D}_h^n$ that $\eta_{D,\mathrm{sp}}^n \leq \texttt{Deref} \cdot \max_{E \in \mathcal{D}_h^n} \eta_{E,\mathrm{sp}}^n$ and that $\eta_{D,\mathrm{sp}}^n < \texttt{Comp} \cdot \texttt{DerefSp} \cdot \texttt{EstTmPrev} \cdot \sqrt{\tau}_n/2/\texttt{NBulkCells}$
    - create a new mesh $\mathcal{D}_h^n$ and interpolate the data onto this mesh
  - **if** $\texttt{Count}$ is a multiple of $\texttt{StepsTmDeref}$ and $\texttt{EstTmPrev} < \texttt{Comp} \cdot \texttt{DerefTm} \cdot \texttt{EstSpPrev}$, set $\tau_n = 3\tau_n$ and $\texttt{LevTmRef} = \texttt{LevTmRef} - 1$
  - set $\mathcal{D}_h^{n+1} = \mathcal{D}_h^n$, $\tau_{n+1} = \tau_n$, and $n = n + 1$

3.5 An adaptive discretization of an instationary nonlinear coupled system allowing to achieve a given precision

In Section 2.6.1, a posteriori error estimates derived in [B4] for the two-phase flow are presented. These estimates also allow to distinguish, estimate separately, and balance the different error sources, combining the ideas of all Sections 3.1, 3.2, and 3.4. In particular, the estimate (2.62) can be further developed as follows. Consider the time step n, the linearization step k (by, e.g., the Newton or the fixed point method), the iterative algebraic solver step i, and the corresponding approximations $(s_{\alpha,h\tau}^{k,i}, p_{\alpha,h\tau}^{k,i})$. Then

$$|||(s_\alpha - s_{\alpha,h\tau}^{k,i}, p_\alpha - p_{\alpha,h\tau}^{k,i})|||_{I_n} \leq \eta_{\mathrm{sp},\alpha}^{n,k,i} + \eta_{\mathrm{tm},\alpha}^{n,k,i} + \eta_{\mathrm{lin},\alpha}^{n,k,i} + \eta_{\mathrm{alg},\alpha}^{n,k,i},$$

where $\eta_{\mathrm{sp},\alpha}^{n,k,i}$ is a *spatial estimator*, $\eta_{\mathrm{tm},\alpha}^{n,k,i}$ a *temporal estimator*, $\eta_{\mathrm{lin},\alpha}^{n,k,i}$ a *linearization estimator*, and $\eta_{\mathrm{alg},\alpha}^{n,k,i}$ an *algebraic estimator*. Consequently, the iterative procedures (iterative linearization and iterative algebraic system solution) on a given time level can be stopped whenever the individual errors drop to the level at which they do not affect significantly the overall error. Similarly, the space and time discretization errors can be equilibrated, adjusted so that they are of similar size. Such a procedure is likely to lead to important computational savings, as performing an excessive number of unnecessary linearization/linear solver iterations and using too fine (with respect to the other components of the error) space or time meshes can be avoided. Many of these concepts are known for long time in the engineering practice; I hope that the present developments can set them in a rigorous framework.

Chapter 4

Inexpensive implementations, relations between different numerical methods, and improvement of approximate solutions by local postprocessing

I present in this chapter various relations and equivalences between different numerical methods, namely in view of achieving inexpensive implementations and developing unified frameworks in the sense described in Section 1.1.3. I also mention the results, often stemming from the a posteriori error estimates of Chapter 2, enabling to obtain improved approximations by local postprocessing. Some results leading to nontraditional a priori analyses are also described.

4.1 Inexpensive implementations and relations between different numerical methods

4.1.1 Inexpensive implementation of the mixed finite element method and its relation to the finite volume method

Let us consider the diffusion model problem (2.1a)–(2.1b). The lowest-order Raviart–Thomas–Nédélec mixed finite element method (see [138] and [121]) for this problem leads to linear algebraic systems of the form

$$\begin{pmatrix} \mathbb{A} & \mathbb{B}^t \\ \mathbb{B} & 0 \end{pmatrix} \begin{pmatrix} U \\ P \end{pmatrix} = \begin{pmatrix} F \\ G \end{pmatrix} \tag{4.1}$$

for flux unknowns U and potential unknowns P of indefinite, saddle-point-type.

There has been a long-standing interest to reduce (4.1) to a system for the potentials P only. The main motivations are to reduce the number of unknowns, to replace the saddle point system (4.1) by, if possible, a symmetric and positive definite one, and to relate the lowest-order mixed finite element method to the finite difference and finite volume ones. A possible solution consists in first using the first block equation of (4.1) to eliminate the unknowns U through

$$U = \mathbb{A}^{-1}(F - \mathbb{B}^t P). \tag{4.2}$$

Note that (4.2) represents a global flux expression (all the fluxes U are expressed from all the potentials P), which includes a solution of a global linear system. Plugging (4.2) into the second block equation of (4.1), one can solve for P the system

$$\mathbb{B}\mathbb{A}^{-1}\mathbb{B}^t P = \mathbb{B}\mathbb{A}^{-1}F - G. \tag{4.3}$$

The matrix $\mathbb{B}\mathbb{A}^{-1}\mathbb{B}^t$ is symmetric and positive definite but the problem is that it tends to be full and cannot be obtained in practice as this would be too expensive. Various approximate numerical quadratures have been used in, e.g., Russell and Wheeler [144], Agouzal et al. [3], Baranger et al. [29], Arbogast et al. [16, 15] to reduce (4.1) into a system of the form

$$\widetilde{\mathbb{S}}\widetilde{P} = \widetilde{H}. \tag{4.4}$$

In these approaches, however, because of the numerical quadratures, the new potentials $\widetilde{P}$ are in general different from those in (4.1) and one cannot recover the exact potentials P. To relations between related numerical methods, we refer to, e.g., Klausen and Russell [106], Droniou et al. [81], Bause et al. [30] and the references therein.

Equivalent, one-unknown-per-element rewriting of (4.1) without any numerical quadrature in the form

$$\bar{\mathbb{S}}\bar{P} = \bar{H}, \tag{4.5}$$

where $\bar{P}$ is a new unknown from which P can be locally recovered, has been achieved in Younès et al. [179], Chavent et al. [63], and Younès et al. [178] by exploiting an equivalence between mixed finite elements and finite volumes. Equivalent, one-unknown-per-element rewriting of (4.1) without any numerical quadrature in the form

$$\mathbb{S}P = H \tag{4.6}$$

has been derived in [170]. In both the above approaches, in contrast to (4.4), one obtains exactly the potentials P of (4.1) (there is no approximation included), and in contrast to (4.3), the matrices $\bar{\mathbb{S}}$ and $\mathbb{S}$ are sparse and locally computable. Intermediately, local flux expressions (enabling to recover the fluxes U of (4.1) on sides of local patches from the potentials P on elements of these patches) have been established in [179, 63, 178, 170].

The first goal of the collaboration [B5] was to give a unified framework, comprising in particular the approaches of [179, 63, 178, 170]. We also testify the closeness/equivalences of the mixed finite element and various finite volume-type methods. The second goal of [B5] was to show via a set of numerical experiments that this approach can indeed lead to inexpensive implementations in the sense of Section 1.1.3. Recall that although (4.5) or (4.6) only gives the potentials $\bar{P}$ or P, the flux unknowns U can be recovered by local flux expressions. In [B5], we also recall that mixed finite elements can easily be defined on general polygonal meshes, via a solution of local Neumann/Dirichlet problems, and the different versions of the discrete maximum principle valid in the mixed finite element method.

4.1.2 A combined finite volume–finite element scheme for degenerate parabolic convection–diffusion–reaction equations on nonmatching grids

The paper [A8] is a follow-up of the work started in [91]. A new scheme allowing to discretize strongly nonlinear, degenerate parabolic convection–diffusion–reaction equations on nonmatching grids is proposed therein. It combines, and uses the tight links between, the cell-centered finite volume and the piecewise affine finite element methods. In this way, the scheme is

fully consistent, locally conservative, and the discrete solution is naturally continuous across the interfaces between the subdomains with nonmatching grids. Moreover, these properties are achieved without introducing any supplementary equations and unknowns or using any interpolation at the interfaces, which allows for an inexpensive implementation; the resulting matrices are positive definite and there is only one unknown per element. The results of a numerical experiment are presented at the end of [A8], using the code TALISMAN [171] where the scheme is implemented.

The tools used in [A8] are to a large extent different from those of Chapters 2 and 3. In particular, in order to show the existence of a unique solution, a Brouwer topopogical degree argument is used, whereas the convergence is shown using a priori energy estimates, estimates on differences of time and space translates for the approximate solution, and the Kolmogorov relative compactness theorem, following Eymard et al. [87, 88, 90].

4.2 Improvement of approximate solutions by local postprocessing

4.2.1 Convergence rate of a postprocessed approximation in the cell-centered finite volume method

The a posteriori error analysis of the cell-centered finite volume method in [A12] for the problem (2.29a)–(2.29b) is carried out for the locally postprocessed potential $\tilde{p}_h$, given, on general polygonal meshes, as the weak solution of the following local Neumann problems:

$$-\nabla\cdot(\mathbf{S}\nabla\tilde{p}_h) = \frac{1}{|K|}\sum_{\sigma\in\mathcal{E}_K} S_{K,\sigma} \quad \forall K\in\mathcal{T}_h, \tag{4.7a}$$

$$(1-\mu_K)\frac{(\tilde{p}_h,1)_K}{|K|} + \mu_K\tilde{p}_h(\mathbf{x}_K) = p_K \qquad \forall K\in\mathcal{T}_h, \tag{4.7b}$$

$$-\mathbf{S}\nabla\tilde{p}_h|_K\cdot\mathbf{n} = \frac{S_{K,\sigma}}{|\sigma|} \qquad \forall\sigma\in\mathcal{E}_K, \quad \forall K\in\mathcal{T}_h. \tag{4.7c}$$

Here, $S_{K,\sigma}$ are the finite volume side fluxes and $\mu_K = 0$ or 1, depending on whether the particular finite volume scheme represents by p_K the approximate mean value on $K\in\mathcal{T}_h$ or the approximate point value in a point $\mathbf{x}_K$ (for simplicity assumed inside K). On simplicial meshes and for $\mu_K = 0$, (4.7a)–(4.7c) reduces to (2.18a)–(2.18b) discussed earlier. The two following results are shown in [A12]: under sufficient regularity of the weak solution p of (2.29a)–(2.29b) ($p\in H^2(\mathcal{T}_h)$) and under appropriate conditions on the given finite volume scheme,

$$\sum_{K\in\mathcal{T}_h}\|\nabla(p-\tilde{p}_h)\|_K^2 \le Ch^2, \tag{4.8a}$$

$$\|p-\tilde{p}_h\|_\Omega^2 \le Ch^2. \tag{4.8b}$$

(4.8a)–(4.8b) are $O(h)$ a priori error estimates for both the energy and $L^2(\Omega)$ norms. Moreover, in the diffusion case,

$$\sum_{K\in\mathcal{T}_h}\|\nabla(p-\tilde{p}_h)\|_K^2 \to 0 \quad \text{as} \quad h\to 0,$$

$$\|p-\tilde{p}_h\|_\Omega^2 \to 0 \quad \text{as} \quad h\to 0,$$

which are convergence results under the minimal regularity ($H_0^1(\Omega)$) of the weak solution p.

4.2.2 Primal formulation-based a priori analysis of the mixed finite element method

The a posteriori error analysis of the mixed finite element method in [A11, A14], see Section 2.2.2, is based on the local postprocessing of the potential (2.18a)–(2.18b) for the lowest-order case or that of Arnold and Brezzi [19] and Arbogast and Chen [13] for the higher-order cases. It turns out that using this postprocessing, the a priori error analysis of mixed finite element methods can also be done, in a quite straightforward way.

In a priori analysis of mixed finite element methods, it is classical and very easy to show that (cf. [A14, Theorem 5.1])

$$|||\mathbf{u}-\mathbf{u}_h|||_* \leq |||\mathbf{u}-I_{\mathbf{V}_h}(\mathbf{u})|||_*, \tag{4.9}$$

where, for $\mathbf{v} \in [L^2(\Omega)]^d$,

$$|||\mathbf{v}|||_* := \|\mathbf{S}^{-\frac{1}{2}}\mathbf{v}\|$$

is the vector energy norm and $I_{\mathbf{V}_h}$ is the mixed finite element interpolation operator onto the flux space $\mathbf{V}_h$. From (4.9), obtaining optimal a priori error estimates for the error in the fluxes $\mathbf{u}_h$ follows by classical results of the interpolation theory. It is for the a priori estimates for the potentials p_h that the not-so-easy-to-show uniform-in-h discrete inf–sup condition is necessary; the estimate for p_h then also takes much less straightforward form than that of (4.9) for $\mathbf{u}_h$.

In [A14], we proceed differently in order to obtain the a priori error estimates for the error in the potentials. Our analysis relies on the postprocessed potential $\tilde{p}_h$. Note in particular that in the lowest-order case, we by (2.18a) and by the definitions of the energy norms have

$$|||p-\tilde{p}_h||| = |||\mathbf{u}-\mathbf{u}_h|||_*.$$

Thus, the a priori error estimate for $|||p-\tilde{p}_h|||$ is immediate from (4.9). For the higher-order cases, [A14, Lemma 5.4] is the key result enabling to proceed similarly as in the lowest-order case and arrive on the final estimate for $|||p-\tilde{p}_h|||$, see [A14, Theorem 5.5]. The L^2-norm a priori estimate for $\|p-\tilde{p}_h\|$ then follows immediately as

$$\|p-\tilde{p}_h\| \leq C|||p-\tilde{p}_h|||$$

by the discrete Friedrichs inequality (A.6), see [A14, Theorem 5.5]. From this last bound, it is immediate to arrive at an L^2-norm a priori estimate for the error in the original potentials p_h, $\|p-p_h\|$, see [A14, Theorem 5.6]. Crucially, the uniform discrete inf–sup condition is not necessary at this step as it is the case in standard analyses. Finally, superconvergence estimates on $\|P_{\Phi_h}(p)-p_h\|$, where P_{Φ_h} stands for the L^2-orthogonal projection onto the potential space Φ_h, can be obtained, see [A14, Theorem 5.7], and therefrom superconvergence estimates on $\|p-\tilde{p}_h\|$ easily follow, see [A14, Theorem 5.8]. The uniform discrete inf–sup condition, not necessary in our analysis, can in fact be shown as a simple consequence of the above results, cf. [A14, Theorem 5.9].

Summarizing, the two main tools of the analysis of [A14] are the local postprocessing and the discrete Friedrichs inequality.

4.2.3 Efficient discretization of the contact between two membranes with a local postprocessing of the actions

In [A1], we have first proposed three different variational formulations of the contact between two membranes (2.40a)–(2.40e): a full mixed one [A1, equation (3.4)], a reduced one [A1, equation (3.11)], and a one including a transformation by the Riesz operator [A1, equation (4.3)]

and analyzed their well-posedness, see [A1, Theorem 3.5]. This analysis has been extended to inhomogeneous Dirichlet boundary conditions in [A2].

The discretization of the contact between membranes appears as less evident. In the first attempt in [A1], we have introduced the Galerkin method for the variational formulation including a transformation by the Riesz operator [A1, equation (4.3)], see [A1, equation (5.4)]. Although an optimal a priori error estimate can be obtained, see [A1, Theorem 6.4 and Corollary 6.7], this approach is computationally quite expensive since it involves not only the approximation of the displacement but also additional discrete unknowns from which the action of one membrane on the other one may be recovered.

The approach of [A2] and [B1] presents an equivalent formulation with the unknowns reduced to the approximations of the displacements of the two membranes only, see [A2, equation (3.4)]. An accurate action of one membrane on the other is then recovered by a local postprocessing, see [A2, equation (4.5)]. Optimal a priori error estimates for both the approximations of the displacements ([A2, Theorem 9]) and the postprocessed action approximation ([A2, Theorem 21]) are also given. The approach of [A2] and [B1] thus gives an inexpensive implementation in the sense of Section 1.1.3.

4.2.4 Local postprocessing of potentials from locally conservative methods

The potential approximation of so-called nonconforming (locally conservative) methods is typically nonconforming, not contained in the energy space; for the model problem (2.1a)–(2.1b), the potential approximation p_h ($\tilde{p}_h$) is typically not contained in the $H^1_0(\Omega)$ space. For completeness, we mention here that the potential reconstruction s_h ($\mathbf{s}_h$, $s_{h\tau}$) used in a posteriori error estimates in [A11, A12, A6, A7, A14, A10] and [B3, B2, B4], cf. the construction of $s_{h\tau}$ in Assumption 2.5.1, may be of independent interest, as it is contained in the energy space; for the model problem (2.1a)–(2.1b), the potential reconstruction s_h in particular belongs to the $H^1_0(\Omega)$ space. Remark that we have presented a potential reconstruction also in the multiscale mortar framework [B3].

4.2.5 Local postprocessing of fluxes from conforming and discontinuous Galerkin methods

The flux approximation is in many numerical methods nonconforming, not contained in the energy space, and not locally conservative; for the model problem (2.1a)–(2.1b), the flux approximation $-\mathbf{S}\nabla p_h$ is typically not contained in the $\mathbf{H}(\mathrm{div},\Omega)$ space and does not satisfy $(-\nabla\cdot(\mathbf{S}\nabla p_h),1)_D = (f,1)_D$ for all elements D of some mesh $\mathcal{D}_h^*$. For completeness, we mention here that the flux reconstruction $\mathbf{t}_h$ ($\underline{\boldsymbol{\sigma}}_h$, $\mathbf{t}_{h\tau}$) used in a posteriori error estimates in [C1, C2], [A6], and [B2] for discontinuous Galerkin methods and in [C4], [A3, A4, A2, A7, A5, A13, A9], and [B1, B4, B2] for conforming finite element/vertex-centered finite volume methods may be of independent interest, as it is contained in the energy space and locally conservative; for the model problem (2.1a)–(2.1b), the flux reconstruction $\mathbf{t}_h$ in particular belongs to the $\mathbf{H}(\mathrm{div},\Omega)$ space and satisfies Assumption 2.2.6. In many cases, much more than Assumption 2.2.6 holds; in the k-th order discontinuous Galerkin method, in particular, we can obtain $\nabla\cdot\mathbf{t}_h = \Pi_k(f)$, where Π_k denotes the L^2-orthogonal projection onto piecewise polynomials on $\mathcal{T}_h$ of degree k, see [C1, Theorem 3.1]. Remark that we have presented a flux reconstruction also in the multiscale mortar framework [B3].

Chapter 5

Perspectives

I describe here shortly the perspectives I see for my research. Quite a few of them are in fact already ongoing works.

5.1 Ongoing projects

The two principal projects I am actually involved in are the GNR MoMaS national research project *A posteriori estimates for efficient calculations and error control in numerical simulations of porous media* and the ERT project *Enhanced oil recovery and geological sequestration of* CO_2*: mesh adaptivity, a posteriori error control, and other advanced techniques.* The goal of these two projects is to develop, for model problems, a posteriori error estimates satisfying as much as possible the five optimal properties of Section 1.1.1 and stopping criteria satisfying as much as possible the four optimal properties of Section 1.1.2 and to derive practical algorithms applicable to nuclear waste repository and multiphase flow simulations, respectively.

5.2 Co-supervision of Ph.D. candidates

In the framework of the GNR MoMaS project, I have a chance to co-supervise the Ph.D. thesis of Nancy Chalhoub, together with Alexandre Ern (Ecole Nationale des Ponts et Chaussées, Marne-la-Vallée) and Toni Sayah (Université Saint-Joseph, Beirut, Lebanon). The subject of this thesis is the development of a general framework for a posteriori error estimation in instationary convection–diffusion–reaction problems. The framework is primarily focused on nonconforming locally conservative methods (the cell-centered finite volume method, the discontinuous Galerkin method, the mixed finite element method) and is derived for the energy norm augmented by a dual norm of the convective derivative following Verfürth [167].

In the framework of the ERT project, I have a chance to co-supervise two Ph.D. theses, together with Daniele Di Pietro (French Petroleum Institute) and Vivette Girault (Laboratoire Jacques-Louis Lions). The first one is that of Soleiman Yousef. In its theoretical part, the goal is to develop optimal a posteriori error estimates, stopping criteria, and adaptive algorithms for the Stefan problem. In its practical part, the goal is to implement these estimates, criteria, and algorithms into the parallel platform Arcane of the French Petroleum Institute. The second Ph.D. thesis is that of Carole Widmer. The subject are a posteriori error estimates for cell-centered finite volume discretizations of two-phase flows, mainly adaptivity with a particular emphasis on front tracking, parallel implementations, and load balancing.

5.3 Ongoing collaborations

There are a couple of collaborations that I am involved in, at various stages of advancement.

Together with Alexandre Ern, we are currently in [86] undertaking theoretical analysis of coupling of the ideas of [A10] and [A5] while proposing and justifying theoretically adaptive inexact Newton discretizations. We are also in [85] interested in relations, equivalences, and inexpensive implementations of discontinuous Galerkin methods.

In a collaboration with Vít Dolejší and Alexandre Ern, we in [77] propose a new framework for a posteriori error estimation for unsteady nonlinear convection–diffusion problems, enabling in particular to obtain local efficiency in both space and time.

Together with Barbara Wohlmuth, we are working on extensions/completions of the results of [B5] to all order mixed finite element methods [172] and to the nonconforming finite element method [173].

With Sorin Pop and Clément Cancès, we are working in [50] on rigorous a posteriori error estimates for two-phase flows.

With Christine Bernardi, Alexandre Ern, and Frédéric Hecht, we are in [39] also working on the extension of flux reconstruction a posteriori error estimates to fourth-order problems.

Finally, with Pavel Jiránek and Zdeněk Strakoš, we investigate stopping criteria for algebraic solvers in the framework of conforming finite element methods [102].

5.4 Intended works

In a longer outlook, I would like to stay in the field of numerical analysis and scientific calculations. I also intend to be active in collaborations with the industry. My personal motivation is to develop algorithms allowing for error control and efficiency in the sense of Section 1.1, which could be applied to real problems in order to advance the current technological limits.

Appendix A

Technical tools

Two important technical tools are used for many of the results of this habilitation. I recall them here for completeness.

A.1 Poincaré, Friedrichs, and trace inequalities

Poincaré, Friedrichs, and trace inequalities play an important role in the theory of partial differential equations.

Let $D \subset \Omega$ be a polygon or polyhedron. The Poincaré inequality states that

$$\|\varphi - \varphi_D\|_D^2 \le C_{\mathrm{P},D} h_D^2 \|\nabla\varphi\|_D^2 \qquad \forall \varphi \in H^1(D), \tag{A.1}$$

where φ_D is the mean of φ over D given by $\varphi_D := (\varphi, 1)_D/|D|$. The constant $C_{\mathrm{P},D}$ can for each convex D be evaluated as $1/\pi^2$, cf. Payne and Weinberger [130] and Bebendorf [32]. To evaluate $C_{\mathrm{P},D}$ for nonconvex elements D is more complicated but it still can be done, cf. Eymard et al. [88, Lemma 10.2] or Carstensen and Funken [53, Section 2].

Let $D \subset \Omega$, $\partial\Omega \cap \partial D \neq \emptyset$. Then the Friedrichs inequality states that

$$\|\varphi\|_D^2 \le C_{\mathrm{F},D,\partial\Omega} h_D^2 \|\nabla\varphi\|_D^2 \qquad \forall \varphi \in H^1(D) \text{ such that } \varphi = 0 \text{ on } \partial\Omega \cap \partial D. \tag{A.2}$$

As long as $\partial\Omega$ is such that there exists a vector $\mathbf{b} \in \mathbb{R}^d$ such that for almost all $\mathbf{x} \in D$, the first intersection of $\mathcal{B}_\mathbf{x}$ and ∂D lies in $\partial\Omega$, where $\mathcal{B}_\mathbf{x}$ is the straight semi-line defined by the origin $\mathbf{x}$ and the vector $\mathbf{b}$, $C_{\mathrm{F},D,\partial\Omega} = 1$, cf. [169, Remark 5.8]. To evaluate $C_{\mathrm{F},D,\partial\Omega}$ in the general case is more complicated but it still can be done, cf. [169, Remark 5.9] or Carstensen and Funken [53, Section 3].

Finally, for a simplex $K \subset \Omega$, the trace inequality states that

$$\|\varphi\|_\sigma^2 \le C_{\mathrm{t},K,\sigma}(h_K^{-1}\|\varphi\|_K^2 + \|\varphi\|_K \|\nabla\varphi\|_K) \qquad \forall \varphi \in H^1(K). \tag{A.3}$$

It follows from Stephansen [148, Lemma 3.12] that the constant $C_{\mathrm{t},K,\sigma}$ can be evaluated as $|\sigma|h_K/|K|$, see also Carstensen and Funken [53, Theorem 4.1] for $d = 2$.

A.2 Discrete Poincaré and Friedrichs inequalities

Recall the Friedrichs and Poincaré inequalities on the whole computational domain Ω, cf. (A.2) and (A.1):

$$\|\varphi\|^2 \le c_\mathrm{F} h_\Omega^2 \|\nabla\varphi\|^2 \qquad \forall \varphi \in H_0^1(\Omega) \tag{A.4}$$

and

$$\|\varphi\|^2 \leq c_{\mathrm{P}} h_\Omega^2 \|\nabla\varphi\|^2 + \tilde{c}_{\mathrm{P}}(\varphi, 1)^2 \qquad \forall\varphi \in H^1(\Omega). \tag{A.5}$$

In numerical approximations, one often works with functions not contained in the spaces $H_0^1(\Omega)$ or $H^1(\Omega)$. Let $W(\mathcal{T}_h)$ be formed by functions locally in $H^1(K)$ on each $K \in \mathcal{T}_h$ such that the mean values of their traces on interior sides coincide. Let also $W_0(\mathcal{T}_h) \subset W(\mathcal{T}_h)$ be such that the mean values of the traces on exterior sides of functions from $W_0(\mathcal{T}_h)$ are equal to zero. These spaces are nonconforming approximations of the continuous ones, i.e. $W_0(\mathcal{T}_h) \not\subset H_0^1(\Omega)$ and $W(\mathcal{T}_h) \not\subset H^1(\Omega)$. Discrete Poincaré and Friedrichs inequalities are the discrete versions of (A.4) and (A.5), valid on the spaces $W_0(\mathcal{T}_h)$ and $W(\mathcal{T}_h)$, respectively. There in particular holds

$$\|\varphi_h\|^2 \leq C_{\mathrm{F}} h_\Omega^2 \sum_{K\in\mathcal{T}_h} \|\nabla\varphi_h\|_K^2 \qquad \forall\varphi_h \in W_0(\mathcal{T}_h),\ \forall h > 0 \tag{A.6}$$

and

$$\|\varphi_h\|^2 \leq C_{\mathrm{P}} h_\Omega^2 \sum_{K\in\mathcal{T}_h} \|\nabla\varphi_h\|_K^2 + \tilde{C}_{\mathrm{P}}(\varphi_h, 1)^2 \qquad \forall\varphi_h \in W(\mathcal{T}_h),\ \forall h > 0, \tag{A.7}$$

where C_{F}, C_{P}, and $\tilde{C}_{\mathrm{P}}$ are generic constants (see [169] for their precise forms). We refer to Eymard et al. [87], Dolejší et al. [78], Knobloch [107], Brenner [45], or to [169] for more details.

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A POSTERIORI ERROR ESTIMATES, STOPPING CRITERIA, AND INEXPENSIVE IMPLEMENTATIONS

for error control and efficiency in numerical simulations

Abstract

This habilitation deals with numerical algorithms for the discretization of linear and nonlinear elliptic and parabolic convection–diffusion–reaction partial differential equations, of the Stokes equation, and of a model variational inequality. The principal focus is on developing algorithms which allow to attain a user-given precision. Moreover, the calculation should be efficient in the sense that as small as possible amount of computational work is needed.

Our principal tool are a posteriori error estimates. We derive them for many classical numerical methods, such as the finite volume, finite element, mixed finite element, and discontinuous Galerkin ones. We often devise unified frameworks, incorporating all these methods. We focus on deriving estimates which would be optimal, i.e., which i) give a guaranteed, fully computable upper bound on the error between the unknown exact solution and the known approximate solution; ii) are locally efficient, i.e., give a local lower error bound; iii) are asymptotically exact, i.e., ensure that the effectivity index (the ratio of the estimated and actual error) goes to one as the computational effort grows; iv) are robust in the sense that the three previous properties hold independently of the parameters and of their variation; and v) which have a small evaluation cost.

Our estimates allow to distinguish, estimate separately, and compare different error sources. One then can stop the different iterative algorithms (iterative linear solvers, iterative nonlinear solvers) whenever the corresponding subsidiary errors drop to the level at which they do not affect significantly the overall error. We can also adjust the calculation parameters (e.g., space meshes and time steps) such that the substantial errors (spatial discretization error, temporal discretization error) are equally distributed and of comparable size. Through such an adaptivity, efficient calculation with error control can be attained.

The last part of this habilitation is dedicated to inexpensive implementations and to the study of the relations between different numerical methods, which in particular allows to develop unified frameworks. We also show how to obtain improved approximate solutions by local postprocessing and present nontraditional a priori analyses.

All the papers forming this habilitation contain a theoretical analysis. Some of them also describe implementations of adaptive algorithms into scientific calculation codes and the majority of them are closely related to applications such as simulations of flow and contaminant transport in porous media, multiphase reservoir flows, or unilateral contact problems.

Key words: second-order convection–diffusion–reaction problem, Stokes problem, monotone nonlinear problem, degenerate parabolic problem, variational inequalities, finite volume method, finite element method, mixed finite element method, discontinuous Galerkin method, nonmatching grids, multiscale, multinumerics, mortar coupling, existence and uniqueness, convergence, a priori error estimate, a posteriori error estimate, iterative methods for linear algebraic systems, iterative linearization, stopping criteria, balancing error components, adaptive mesh refinement, efficient calculation, error control, relations between different methods, local flux expression, local postprocessing, unified framework, robustness, flow and contaminant transport, multiphase flows, porous media, unilateral contact, elastic membranes

AMS subject classifications: 35J20, 35K65, 46E35, 65M12, 65M15, 65M60, 65N15, 65N30, 74K15, 74M15, 76M10, 76M12, 76S05