UNIVERSITE PIERRE ET MARIE CURIE – PARIS 6

Habilitation à diriger des recherches

spécialité mathématiques appliquées

présentée par

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Sujet :

ESTIMATIONS D'ERREUR A POSTERIORI, CRITERES D'ARRET ET IMPLEMENTATIONS PEU COUTEUSES

pour contrôle d'erreur et efficacité dans des simulations numériques

Soutenue le 13 décembre 2010 devant le jury composé de :

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Avant-propos

Cette habilitation résume les travaux auxquels j'ai participé en tant que maître de conférences au Laboratoire Jacques-Louis Lions, Université Pierre et Marie Curie à Paris et antérieurement en tant que post-doctorant au Centre national de la recherche scientifique à Orsay.

Le sujet principal de cette habilitation est l'analyse numérique et, accessoirement, le calcul scientifique. La majorité des articles contient des résultats théoriques : analyse de problèmes continus, démonstrations de convergence, estimations d'erreur a priori et a posteriori et proposition et étude d'algorithmes adaptatifs. J'ai également participé au développement de codes de calcul scientifique.

Beaucoup de résultats présentés dans cette habilitation sont étroitement liés ou motivés par des calculs pratiques et des problèmes réels. Pendant mon post-doctorat, j'ai collaboré avec la société HydroExpert sur des simulations d'écoulements et transport de contaminants en milieu poreux, développant un code de calcul adaptatif. A l'Université Pierre et Marie Curie, j'ai eu la chance d'être inclus dans le projet *Estimations d'erreur a posteriori pour des calculs efficaces et contrôle d'erreur dans des simulations numériques du milieu poreux* dans le cadre du projet du Centre national de la recherche scientifique GNR MoMaS *Modélisations mathématiques et simulations numériques liées aux problèmes de gestion des déchets nucléaires*. Ce projet comporte des interactions avec le CEA, le Commissariat à l'énergie atomique. Finalement, c'est avec plaisir pour moi de collaborer avec l'IFP, l'Institut français du pétrole, à travers le projet ERT *Récupération d'huile assistée et séquestration géologique du* CO_2 *: adaptation de maillage, contrôle d'erreur a posteriori et autres techniques avancées.*

Je crois sincèrement que les mathématiques et en particulier l'analyse numérique devraient être appliquées aux problèmes réels dans le but d'avancer les limites technologiques. J'espère que les résultats présentés dans cette habilitation y contribueront...

Remerciements

Mes premiers remerciements vont aux tous les membres du Laboratoire Jacques-Louis Lions. Je suis en particulier très reconnaissant à son directeur, Yvon Maday, qui m'a accueilli les bras ouverts. Le Laboratoire Jacques-Louis Lions est un endroit magnifique à travailler, avec des conditions scientifiques parfaites, un environnement très stimulant, beaucoup d'événements variés au programme, un nombre extraordinaire de gens que j'apprécie profondément tant sur le plan scientifique que sur le plan humain et – ce que j'apprécie personnellement beaucoup – une atmosphère très amicale.

Je remercie très sincèrement Roland Becker, Serge Nicaise et Rüdiger Verfürth d'avoir accepté d'être mes rapporteurs et de tous leurs avis exprimés dans les rapports. Et je suis vraiment honoré qu'Alexandre Ern, Raphaèle Herbin, Yvon Maday, Rolf Stenberg et Zdeněk Strakoš ont accepté de participer à mon jury.

Mes remerciements les plus chaleureux sont adressés à Alexandre Ern. Pour ces heures, jours, semaines et mois que nous avons passés ensemble sur la ligne enthousiaste entre le connu et l'inconnu. Pour ces nombreux essais, échecs, mais aussi succès que nous avons pu célébrer à la fin d'un long chemin... Alexandre, merci pour tout et merci aussi pour avoir relu ce manuscrit !

Je suis très reconnaissant à Christine Bernardi, Faker Ben Belgacem et Adel Blouza. C'est grâce à eux que j'ai pu commencer à découvrir le monde des inégalités variationnelles.

Je suis très content d'avoir eu l'occasion d'interagir avec tous les participants du projet MoMaS ; merci à Linda El Alaoui, merci à Annette Stephansen, merci à Pascal Omnes, Christophe Le Potier et Philippe Montarnal et merci à Jean Roberts et Jérôme Jaffré.

C'est un grand plaisir de travailler sur le projet ERT avec l'IFP, l'Institut français du pétrole. Je voudrais exprimer ma reconnaissance à Roland Masson et Daniele Di Pietro en particulier.

Je me sens très enrichi par toutes mes visites à Austin. Je voudrais remercier Gergina Pencheva, Todd Arbogast, Tim Wildey, Guangri Xue et tous les membres au Centre des modélisations du sous-sol, pour des discussions incalculables sur les éléments finis mixtes, multi-échelles et joints. Mes remerciements particuliers vont à Mary Wheeler pour tout de ci-dessus mais aussi pour la visite de son ranch et l'inoubliable chasse aux sangliers...

J'ai des sentiments particuliers pour mon pays natal. C'était un honneur et plaisir pour moi de travailler avec Zdeněk Strakoš et Pavel Jiránek, jusqu'au jour où nous avons enfin arrêté le solveur ! Et c'est toujours une joie pour moi de travailler avec Vít Dolejší, sur n'importe quoi qui soit discontinu.

Mes remerciements très chaleureux vont à Barbara Wohlmuth pour toutes les heures et jours des discussions passionnantes, finalement pas seulement sur les mathématiques.

J'ai beaucoup profité de mon séjour en Finlande. Je voudrais remercier à Rolf Stenberg pour cette expérience, et, bien sur, avant tout pour le travail sur le problème de Stokes. Et mille mercis à Antti Hannukainen, notre guru de programmation.

J'ai beaucoup apprecié (et j'espère qu'elle continuera) notre collaboration avec Sorin Pop et Clément Cancès. Vive les écoulements diphasiques !

Je suis très reconnaissant à Danielle Hilhorst pour son soutien pendant mon post-doctorat et pour ses encouragements constants. Je dois beaucoup à Robert Eymard qui m'a appris tant de choses. Je tiens aussi à remercier à chacun à HydroExpert pour mes débuts ; en particulier à Lionel Demongodin pour son soutien et à Marc Bonnet pour toutes les discussions sur l'arrière-plan hydrogéologique. Et merci beaucoup à Libor Inovecký de Prague. Nous avons passé beaucoup de temps sur les concepts de programmation du code TALISMAN (et un peu

sur la guitare aussi quand-même...). Mes remerciements sincères vont à chacun à l'Université Technique à Liberec, Jiří Maryška, Jan Šembera, Otto Severýn et Milan Hokr en particulier.

J'ai des souvenirs très agréables de mon séjour au Japon chez Mayan Mimura. Cette expérience incluait la programmation avec Matlab, des systèmes de réaction–diffusion, et bien sûr la vie japonaise.

C'est toujours un plaisir personnel pour moi de discuter avec Jean-François Maître. Je souhaite d'avoir autant d'énergie et d'enthousiasme quand j'aurai son âge !

Je voudrais remercier particulièrement Marie Postel pour son aide gentille avec la relecture de ce manuscrit.

Mes souvenirs sympathiques vont ensuite au CEMRACS 2007. Merci aux organisateurs ! Et merci aux membres de mon projet étudiant, Mariana, Ibrahim et Radek, pour tout le travail qu'on a fait et pour tout l'amusement qu'on a eu.

L'une de mes plus grandes sources de mon bonheur est le stimulus que j'obtiens de mes étudiants. Merci Nancy, merci Carole, merci Soleiman. Et bonne chance pour vos thèses !

C'est un honneur pour moi et je suis très enchanté de pouvoir co-organiser le groupe de travail des méthodes numériques au Laboratoire Jacques-Louis Lions. J'ai beaucoup appris de Vivette Girault et d'Olivier Pironneau et je voudrais exprimer toute ma gratitude d'avoir eu cette chance.

Une dernière itération : merci à toutes les secrétaires en toutes ces destinations variées. Je n'aurais jamais pu voyager sans eux : merci à Connie Baxter, Tuula Donskoi, Lindsey Maddox et Brit Steiner.

Et là je suis, à la fin. Sur mes trésors personnels. Je n'aurais jamais pu achever les résultats de cette habilitation sans le support de ma fiancée Martina et sa compréhension infinie pour rester tard au travail, voyager à une conférence, être à l'étranger... Et je ne serai là où je suis sans ma famille et sans mes amis...

A Martina

A mes parents

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Chapitre 1

Introduction

1.1 Introduction générale et terminologie

Un grand nombre de phénomènes environnementaux et physiques sont décrits par des équations aux dérivées partielles. Hélas, dans la plupart des cas, il n'est pas possible de trouver des *solutions exactes*, analytiques de ces équations. Par conséquent, des méthodes numériques, c'est-à-dire des algorithmes mathématiques évalués à l'aide d'ordinateurs, sont utilisées pour des simulations.

A part des cas très particuliers, les méthodes numériques fournissent seulement des *solutions approchées*, le plus souvent des fonctions définies dans un espace de dimension finie, différentes des solutions exactes. Deux questions d'une importance essentielle sont :

1. Quelle est la grandeur de l'erreur entre les solutions exacte et approchée ?
2. Où l'erreur est-elle localisée ?

Les réponses à ces questions peuvent être décisives dans la construction des ponts et barrages, la fabrication des voitures et avions, les prévisions de la météo, l'exploitation du pétrole et du gaz naturel, la dépollution des sols et océans, dans la pharmacie, les techniques avancées dans la santé publique, les simulations de la dynamique des populations, les prévisions économiques et financières etc... En effet la décision est souvent prise sur la base du résultat numérique ; cf., par exemple, Ladevèze et Moës [112], Babuška et Oden [23] et Oden et al. [128]. Dans cette direction de raisonnement, le but final est de concevoir des algorithmes où :

3. La précision donnée avant le début de la simulation est obtenue à la fin de la simulation (*contrôle de l'erreur*).
4. La quantité de travail nécessaire est la plus petite possible (*calcul efficace*).

Nous décrivons ci-dessous plusieurs axes permettant de contribuer à la satisfaction de ce but : les estimations d'erreur a posteriori, les critères d'arrêt et les discrétisations adaptatives et les implémentations peu coûteuses.

1.1.1 Estimations d'erreur a posteriori

Traditionnellement, la qualité des solutions numériques approchées est exprimée à l'aide des *estimations d'erreur a priori*. Ces estimations peuvent être évaluées avant le début du calcul et donnent des bornes sur la différence entre la solution exacte et la solution approchée. Cette borne dépend typiquement de la taille des mailles (qui tend vers zéro avec le raffinement du

maillage) et une constante inconnue qui dépend de la solution exacte. Ces estimations sont utilisées afin de justifier théoriquement la méthode numérique concernée. Malheureusement, en pratique la borne supérieure ne peut quasiment jamais être évaluée et ne peut donc pas donner une réponse aux deux questions énumérées ci-dessus et de servir à réaliser les deux exigences énumérées ci-dessus.

Le but des *estimations d'erreur a posteriori* est de donner des bornes sur l'erreur entre l'approximation numérique et la solution exacte inconnue qui peuvent être calculées en pratique, une fois que la solution approchée est connue, cf. Verfürth [161], Ainsworth et Oden [9], Babuška et Strouboulis [26], Neittaanmäki et Repin [122], Han [96], ou Repin [141]. Par conséquent, en principe, les estimations d'erreur a posteriori peuvent être utilisées pour donner des réponses aux questions 1 et 2 ci-dessus. On peut donc aussi espérer pouvoir construire des algorithmes répondant aux exigences des points 3 et 4 ci-dessus.

Pour les estimations d'erreur a posteriori, on peut formuler les propriétés suivantes, décrivant une estimation optimale :

- **i)** fournir une borne supérieure d'erreur entre la solution exacte et approchée qui soit entièrement (sans aucune constante inconnue) calculable à partir de la solution approchée (*borne supérieure garantie*) ;
- **ii)** donner une expression de cette estimation localement, par exemple dans chaque élément du maillage, et garantir que cette estimation est aussi localement une borne inférieure de l'erreur à une constante multiplicative près (*efficacité locale*) ;
- **iii)** garantir que l'index d'efficacité, donné comme le rapport entre l'erreur estimée et l'erreur actuelle, tend vers 1 en augmentant le coût du calcul (*exactitude asymptotique*) ;
- **iv)** garantir les trois propriétés précédentes indépendamment des paramètres et de leur variation (*robustesse*) ;
- **v)** donner des estimations pouvant être évaluées localement (*coût négligeable*).

La propriété **i)** permet de donner une borne d'erreur supérieure entièrement calculable, c'est-à-dire, de répondre à la question 1. La propriété **ii)** permet de prédire la localisation d'erreur et donc de répondre à la question 2. Ayant connaissance de la localisation de l'erreur, on peut concentrer plus d'efforts dans cette partie du domaine de calcul. En pratique le maillage est raffiné là où l'erreur est grande, ce qui introduit la notion de *raffinement adaptatif du maillage*. La propriété **iii)** assure l'optimalité de la borne supérieure ; si l'erreur est petite et si l'estimateur prédit une valeur élevée, il peut vérifier quand même la propriété **i)** ; il n'est cependant pas très utile en pratique car il surestime beaucoup l'erreur. La propriété **iv)** est l'une des plus importantes en pratique. Dans des problèmes réels, les paramètres et coefficients (diffusivité, réactivité, convection, grandeur de la non linéarité, taille relative des échelles d'espace et du temps) peuvent varier sur plusieurs ordres de grandeur. Un estimateur qui satisfait la propriété **iv)** assure que les résultats vont être de la même qualité dans toutes les situations. Enfin, la propriété **v)** garantit que le coût d'évaluation va être beaucoup plus petit que le coût requis pour obtenir la solution approchée elle-même (rappelons que d'habitude, un problème global doit être résolu afin d'obtenir la solution approchée).

Nous présentons au paragraphe 2.1 ci-dessous l'état de l'art des estimations a posteriori.

1.1.2 Critères d'arrêt et discrétisations adaptatives

Un algorithme numérique inclut typiquement plusieurs procédures itératives. Par exemple, pour un problème non linéaire instationnaire, il y a d'habitude une boucle sur les pas de temps,

des itérations de linéarisation et, dans le cas où un solveur algébrique itératif est utilisé, des itérations du solveur algébrique, cf. Szabó et Babuška [153], Quarteroni et Valli [137], Babuška et Strouboulis [26], Ern et Guermond [82] et Han [96]. Afin de satisfaire les critères 3 et 4 énoncés ci-dessus, on peut envisager, à chaque moment du calcul :

i) distinguer et estimer séparément les différentes composantes de l'erreur (*identification et séparation des composantes d'erreur*) ;

ii) classifier les composantes de l'erreur en deux groupes : *les composantes substantielles de l'erreur* (essentielles pour le calcul, les erreurs qui vont être toujours présentes (par exemple l'erreur de discrétisation en espace, l'erreur de discrétisation en temps)) et les *composantes subsidiaires de l'erreur* (secondaires pour le calcul, les erreurs qui sont en général très petites ou même nulles pour un nombre suffisant d'itérations, par exemple l'erreur de linéarisation, l'erreur du solveur algébrique linéaire) ;

iii) arrêter les différents algorithmes itératifs au moment où les erreurs subsidiaires correspondantes diminuent en deçà du niveau où elles n'affectent plus l'erreur totale (*critères d'arrêt*) ;

iv) ajuster les paramètres du calcul (par exemple les maillages en espace ou les pas de temps) de telle sorte que les erreurs substantielles soient distribuées de façon équilibrée et de grandeurs comparables (*équilibrage des composantes d'erreur*).

Pour conclure cette petite introduction, citons Baxter et Iserles [31, p. 273] : « Le but d'un calcul n'est pas de produire une solution avec l'erreur la plus petite possible, mais de produire, de façon fiable, robuste et abordable, une solution avec une précision spécifiée par l'utilisateur. » Par conséquent, les erreurs substantielles commises aux différentes étapes du calcul devraient être équilibrées et les erreurs subsidiaires petites ; voir par exemple, Babuška [21], Han [95], Becker et al. [35], Ladevèze et Moës [113, 112], Ladevèze [110], Babuška et Oden [23], Oden et al. [128], Strakoš et Tichý [150] et Chaillou et Suri [61, 62]. Le respect des quatre propriétés **i)**–**iv)** ci-dessus assurera un calcul efficace permettant le contrôle de l'erreur au sens du paragraphe 1.1.

1.1.3 Implémentations, relations entre différentes méthodes numériques et post-traitement local

Comme on l'a dit plus haut, l'une des questions centrales en simulations numériques est celle de l'efficacité des calculs. Une méthode numérique peut souvent être implémentée de plusieurs façons différentes, menant au même résultat. Nous allons appeler de telles implémentations des *implémentations équivalentes*. Si on trouve une façon moins coûteuse que les autres en terme de temps du calcul, on peut gagner beaucoup en terme d'efficacité du calcul. Par exemple, influencer les propriétés de la matrice finale (symétrie, positivité, nombre d'inconnues, nombre d'éléments non nuls sur chaque ligne, nombre de conditionnement) est une voie pour arriver à une *implémentation peu coûteuse*.

Les différentes implémentations d'une même méthode numérique sont étroitement liées aux méthodes apparemment différentes qui peuvent néanmoins être montrées équivalentes dans le sens où le même résultat peut être obtenu à la fin des calculs. Nous allons appeler de telles méthodes *méthodes numériques équivalentes*. Prenons l'exemple de la méthode des volumes finis centrés par sommet et la méthode des éléments finis. La méthode des volumes finis est localement conservative par construction, alors que la méthode des éléments finis n'est pas localement conservative par construction. Il se trouve, néanmoins, que, sous certaines

conditions, ces deux méthodes sont équivalentes (le même résultat peut être obtenu à la fin des calculs). La relation d'équivalence permet en particulier de reconstruire des flux localement conservatifs à partir de la solution éléments finis (de tels flux ne sont pas disponibles au premier coup d'œil).

Certains de ces concepts sont en fait étroitement liés aux techniques utilisées en estimations d'erreur a posteriori. Ici un *post-traitement local*, c'est-à-dire une construction locale des approximations améliorées, joue un rôle central. En estimations d'erreur a posteriori, il est courant de post-traiter localement des potentiels conformes et/ou des flux conformes et localement conservatifs. Les termes *reconstruction du potentiel* et *reconstruction du flux* sont aussi utilisés.

Nous voudrions enfin mentionner que les techniques évoquées ci-dessus permettent également de mener des analyses a priori non traditionnelles.

1.2 Liste des articles de cette habilitation

Les articles de cette habilitation sont organisés en trois groupes distincts : articles dans des journaux internationaux avec un comité de lecture, articles soumis aux journaux internationaux avec un comité de lecture (et un article important, actuellement en préparation) et des articles courts, notes et actes de congrès.

Le premier groupe contient des articles de quelques dizaines de pages, publiés ou acceptés pour publication dans des journaux internationaux avec un comité de lecture. Signalons cependant une exception à la règle. L'article [A3] a été rédigé à partir d'un projet étudiant effectué pendant le Centre d'été en mathématiques CEMRACS 2007 et publié dans *ESAIM : Proceedings*. Il se trouve inclus dans le premier groupe car il s'agit d'un travail de recherche original qui n'a pas été publié par ailleurs. Les codes de référence à ce groupe, qui forme la base de cette habilitation, commencent par la lettre « A ».

Le deuxième groupe est formé d'articles soumis pour publication dans des journaux internationaux avec un comité de lecture, et comprend également un article actuellement en préparation. Ces articles sont inclus dans cette habilitation car ils comportent, à mon avis, beaucoup de résultats importants. Les codes de référence à ce groupe commencent par la lettre « B ».

Le dernier et troisième groupe comprend des articles courts, des notes et des actes de congrès. Ces articles ont servi pour présenter des idées qui ont été développées ultérieurement dans l'un des articles du premier groupe. Les codes de référence à ce groupe commencent par la lettre « C ». Ils figurent dans cette bibliographie uniquement pour qu'elle présente l'intégralité de mes publications.

Aucun article présenté ci-dessous n'a fait partie ou est directement lié à ma thèse de doctorat.

Après chaque article, je liste entre crochets les numéros des pages où ils est cité.

1.2.1 Articles dans des journaux avec un comité de lecture

[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. [17, 18, 22, 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. [21, 22, 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, 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. [17, 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. [17, 18, 19, 20, 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. [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. [17, 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. [21, 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. [17, 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. [17, 18, 19, 20, 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. [17, 18, 22, 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. [17, 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. [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. [17, 22, 32, 33, 62, 63]

1.2.2 Articles soumis pour publication dans des journaux avec un comité de lecture

[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, soumis pour publication, 2010. [17, 18, 21, 22, 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, soumis pour publication, 2010. [17, 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, soumis pour publication, 2010. [17, 19, 20, 33, 34, 35, 55, 63]

[B4] Vohralík, M. A posteriori error estimates, stopping criteria, and adaptivity for two-phase flows. En préparation, 2010. [17, 19, 21, 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, soumis pour publication, 2010. [21, 60, 66]

1.2.3 Articles courts, notes et actes de congrès

[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. [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. [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. [17, 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. [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. [17, 28]

1.3 Contributions principales de cette habilitation

J'associe ici les articles, prépublications et notes avec les trois axes introduits au paragraphe 1.1. Dans toutes les listes ci-dessous, les travaux sont triés par date.

Comme décrit dans l'avant-propos, la majorité de ces articles contient des résultats théoriques : analyse des problèmes continus, démonstrations de convergence, estimations d'erreur a priori et a posteriori et conceptions et études des algorithmes adaptatifs. Beaucoup de ces résultats sont, cependant, motivés ou directement liés aux demandes pratiques. Ces dernières incluent la simulation des déchets radioactifs nucléaires dans le cadre du projet MoMaS *Estimations d'erreur a posteriori pour des calculs efficaces et contrôle d'erreur dans des simulations numériques du milieu poreux* et la simulation des écoulements multiphasiques dans le cadre du projet ERT *Récupération d'huile assistée et séquestration géologique du* CO_2 *: adaptation de maillage, contrôle d'erreur a posteriori et autres techniques avancées*. Certains de ces articles présentent aussi des algorithmes faisant partie de codes de calcul développés.

1.3.1 Estimations d'erreur a posteriori

Aussitôt après ma thèse de doctorat, le sujet principal de mes recherches a été l'analyse a posteriori, cf. l'introduction du paragraphe 1.1.1. Mes contributions sur ce thème ont été les articles [A11, A12, A3, A1, A4, A6, A7, A14, A10, A5, A13, A9], les prépublications [B1, B3, B2, B4] et les notes [C3, C1, C4, C5, C2]. Avec mes coauteurs, j'ai développé des estimations d'erreur a posteriori pour différents problèmes et différentes méthodes numériques qui vérifient aussi bien que possible les cinq propriétés optimales du paragraphe 1.1.1. En particulier, je me suis concentré sur des estimations qui sont simultanément garanties et robustes, et ceci aussi pour des problèmes instationnaires and non linéaires. J'ai également travaillé sur des cadres unifiés. A ma connaissance, les résultats de ce type sont très rares voire inexistants dans la littérature, cf. l'état de l'art des estimations a posteriori donné au paragraphe 2.1 ci-dessous. Ces contributions font le sujet du chapitre 2.

Problèmes stationnaires linéaires

J'ai tout d'abord étudié l'équation de diffusion stationnaire linéaire (l'équation de Laplace ou l'équation de diffusion avec un coefficient de diffusion inhomogène et anisotrope) discrétisée par la méthode des éléments finis continus affines par morceaux (cf. Ciarlet [67]), en [C4] et [A3, A13]. Des résultats similaires pour la méthode de Galerkin discontinue sont données dans [C1, C2] et [A6] et pour la méthode des volumes finis centrés par maille et sommets dans [C5] et [A13]. L'idée principale de ces développements remonte à l'égalité de Prager–Synge [136]. La première intention dans ces travaux est d'obtenir des estimations vérifiant la propriété **i)** du paragraphe 1.1.1. Il s'agit d'assurer que l'estimation donne une borne supérieure d'erreur garantie, sans aucune constante générique inconnue, de telle sorte que l'erreur totale de ces différentes discrétisations numériques soit contrôlée. Accessoirement, on essaie de vérifier au plus la propriété **iii)** (les indices d'efficacité obtenus varient en moyenne entre 1.1 et 1.4). De plus, dans [A13], j'ai réussi à donner une estimation entièrement robuste par rapport aux discontinuités dans le tenseur de diffusion, c'est-à-dire une estimation vérifiant la propriété **iv)**. Toutes les estimations ci-dessus vérifient les propriétés **ii)** et **v)** du paragraphe 1.1.1.

L'article [A13] contient une comparaison systématique des méthodes des différences finies, des éléments finis affines par morceaux et des volumes finis centrés par maille et par sommet pour un problème stationnaire linéaire de diffusion avec un coefficient de diffusion inhomogène et anisotrope. Les relations/équivalences entre ces différentes méthodes ont été utilisées en [A13] afin de présenter les estimations d'erreur a posteriori dans un cadre unifié. Dans [C2], [A6] et en partie dans [A13], nous avons pu aussi prendre en compte des maillages généraux non coïncidants. Les détails sur tous ces développements sont donnés au paragraphe 2.2.1.

Un cadre unifié pour des estimations d'erreur a posteriori optimales vérifiant les cinq propriétés optimales du paragraphe 1.1.1 est proposé dans [A14]. Ce cadre est a priori développé pour différentes familles et ordres de la méthode des éléments finis mixtes mais il s'applique à n'importe quelle méthode localement conservative. Dans ce cadre présenté au paragraphe 2.2.2, nous avons obtenu dans la prépublication récente [B3] trois autres extensions. Dans un premier temps, nous montrons que différentes méthodes numériques (éléments finis mixtes, éléments de Galerkin discontinus, volumes finis) peuvent être utilisées dans différentes parties du domaine de calcul (*multi-numérique*). Dans un deuxième temps, la *technique des joints* peut être utilisée. Dans un dernier temps, la discrétisation peut être faite dans une *formulation multi-échelle*, permettant la décomposition du problème en problèmes à l'échelle h, posés dans des sous-domaines, et à l'échelle H, posés sur l'interface. Une des estimations proposées dans [B3] est robuste par rapport aux échelles multiples, c'est-à-dire par rapport au ratio H/h, sous l'hy-

pothèse d'une régularité suffisante de la solution exacte. Ces contributions sont discutées en détail au paragraphe 2.2.3 ; l'utilisation de ces résultats pour une stratégie adaptative, suivant l'idée de Wheeler et Yotov [175], est décrite dans les paragraphes 1.3.2 et 3.3.

Le dernier article dédié à l'équation de diffusion stationnaire linéaire est [A10]. La discrétisation d'une telle équation conduit à la résolution d'un système d'équations linéaires algébriques. Tous les résultats ci-dessus (en même temps que la plupart des résultats de la littérature) sont basés sur l'hypothèse que ce système linéaire est résolu de façon exacte. Très souvent, ceci n'est pas le cas en pratique. On utilise soit un solveur linéaire direct et dans ce cas les erreurs numériques d'arrondi peuvent être importantes, soit un solveur linéaire itératif qu'on arrête avant que la convergence (exacte) ait été atteinte. Le premier résultat de [A10] propose des estimations d'erreur a posteriori qui permettent de prendre en compte l'erreur dans la résolution du système algébrique linéaire. En plus, dans cet article, l'efficacité (locale) est démontrée. Il en découle que notre estimation d'erreur a posteriori peut être utilisée pour le raffinement adaptif du maillage en tenant compte également de l'erreur algébrique. Ce résultat est l'objet du paragraphe 2.2.4. Il peut aussi par la suite être utilisé comme un critère d'arrêt pour des solveurs itératifs algébriques, voir paragraphes 1.3.2 et 3.1.

Nous avons démontré, avec mes étudiants, une extension des résultats précédents au cas d'une équation de réaction–diffusion singulièrement perturbée en mettant l'accent sur la robustesse – la propriété **iv)**. Nous avons obtenu dans [A4] des estimations robustes par rapport au terme de réaction. Cette contribution est discutée en détail au paragraphe 2.2.5. J'ai par la suite étudié, toujours dans le cadre stationnaire linéaire, l'équation de convection–diffusion–réaction. Les premiers résultats de [A11, A12] et [C3] vérifient les propriétés **i)** et **ii)**, **iii)** (de façon approchée) et **v)**, mais ne vérifient pas la propriété **iv)**. La robustesse manquante a été obtenue dans la collaboration [A6], en ayant remplacé la norme d'énergie par une norme composée de la norme d'énergie augmentée par une norme duale de la dérivée convective, suivant Verfürth [168]. Ces contributions sont discutées en détail au paragraphe 2.2.6.

La dernière extension dans le cas stationnaire linéaire est au cas du problème de Stokes. Nous l'avons menée dans [B2]. Un cadre unifié est développé dans cette référence, voir le paragraphe 2.2.7. Il contient différentes méthodes d'éléments finis conformes et conformes stabilisés, la méthode de Galerkin discontinue, la méthode de Crouzeix–Raviart non conforme, la méthode des éléments finis mixtes et une classe générale de méthodes des volumes finis.

Inégalités variationnelles stationnaires

Avec mes collaborateurs, j'ai aussi eu l'occasion de travailler sur des inégalités variationnelles, plus particulièrement sur le contact entre deux membranes. Nous avons d'abord développé, dans [A1], un modèle pour le contact entre deux membranes, en montrant qu'il est bien posé et en réalisant son analyse d'erreur a priori. Nous avons également dérivé dans ce travail une estimation d'erreur a posteriori de type par résidu. Cette estimation ne vérifie pas la propriété **i)**. En plus, la propriété **ii)** n'est pas vérifiée de façon optimale. Nous avons réussi à améliorer ces deux points et à donner des estimations garanties et localement efficaces (sauf pour un terme numériquement négligeable) dans [B1]. Nous renvoyons au paragraphe 2.3.1 pour plus de détails.

Problèmes stationnaires non linéaires

Nous avons étudié des estimations d'erreur a posteriori pour un problème stationnaire non linéaire monotone du second ordre en [A5]. Nous avons réussi à obtenir les cinq propriétés optimales (l'exactitude asymptotique est seulement approximative) ; les estimations obtenues sont

en particulier garanties et robustes par rapport à la grandeur de la non linéarité pour l'erreur mesurée comme la norme duale du résidu. Ce résultat est décrit au paragraphe 2.4.1. L'utilisation de ces résultats comme un critère d'arrêt adaptatif du solveur non linéaire est décrit dans les paragraphes 1.3.2 et 3.2.

Problèmes instationnaires linéaires

Nous avons également, avec mes collaborateurs, commencé à travailler sur des problèmes instationnaires linéaires. En particulier, nous avons développé dans [A7] un cadre unifié pour l'estimation d'erreur a posteriori pour l'équation de la chaleur. Des estimations donnant une borne supérieure garantie sur l'erreur mesurée dans la norme d'énergie augmentée par la norme duale de la dérivée en temps, aussi bien que des bornes inférieures d'erreur, locales en temps mais globales en espace, ont été dérivées sous deux conditions simples. Nous avons montré par la suite comment vérifier ces conditions pour la méthode de Galerkin discontinue, pour différentes méthodes de volumes finis et pour la méthode des éléments finis mixtes en espace et la méthode d'Euler rétrograde en temps ; les extensions aux méthodes des éléments finis conformes et non conformes en espace sont aussi présentées. Ce résultat est décrit au paragraphe 2.5.1.

En [A9], le résultat précédent est étendu au cas d'une équation de convection–diffusion–réaction instationnaire linéaire. Une borne supérieure garantie pour la norme d'énergie est obtenue et suivant l'approche de Verfürth [167], une borne inférieure robuste par rapport à la dominance par la convection est démontrée pour une norme duale. Nous renvoyons au paragraphe 2.5.2 pour plus de détails. De plus, un algorithme adaptatif peut être construit en se basant sur ces résultats, cf. paragraphes 1.3.2 et 3.4.

Problèmes instationnaires non linéaires

Enfin, le dernier résultat sur les estimations a posteriori de [B4] est donné pour le modèle d'écoulement diphasique, un système couplé des équations instationnaires non linéaires de convection–diffusion. Ce résultat a été obtenu dans le cadre du projet ERT entre le LJLL et l'IFP, l'Institut français du pétrole. Dans un cadre unifié comme celui de ci-dessus, il donne une borne supérieure garantie sur l'erreur mesurée par la norme duale du résidu. Les détails sont donnés au paragraphe 2.6.1. Par ailleurs, en combinant les approches de [A10, A5, A7], un algorithme entièrement adaptatif au sens du paragraphe 1.1.2 peut être construit, voir paragraphes 1.3.2 et 3.5.

1.3.2 Critères d'arrêt et discrétisations adaptatives

Un autre sujet de recherche que j'ai abordé au cours de ces dernières années, étroitement lié aux estimations d'erreur a posteriori, a été les critères d'arrêt pour des solveurs linéaires et non linéaires itératifs et des discrétisations entièrement adaptatives, cf. l'introduction au paragraphe 1.1.2. Mes contributions sur ce thème sont contenues dans les articles [A10, A5, A9] et les prépublications [B3, B4]. Le but est de développer des critères d'arrêt qui satisfassent aussi bien que possible les quatre propriétés optimales du paragraphe 1.1.2 et de construire des algorithmes qui permettent un calcul efficace et un contrôle de l'erreur au sens du paragraphe 1.1. Ces travaux incluent les critères d'arrêt pour les solveurs algébriques linéaires, critères d'arrêt pour les solveurs non linéaires, l'équilibrage des composantes d'erreur dans les discrétisations par des joints, l'équilibrage des erreurs en espace et en temps pour les problèmes instationnaires et aussi une discrétisation entièrement adaptative d'un système instationnaire non linéaire couplé permettant d'obtenir une précision donnée. Cependant, je n'essaie pas de prouver l'optimalité

de ces algorithmes, comme c'est le cas par exemple dans Stevenson [149] ou Cascon et al. [59] pour des problèmes de diffusion modèles. Ces contributions sont le sujet du chapitre 3.

Critères d'arrêt pour des solveurs algébriques linéaires

Des critères d'arrêt pour des solveurs algébriques linéaires, basés sur des estimations d'erreur a posteriori et développant les idées de, par exemple, Babuška [21], Becker et al. [35] et Strakoš et Tichý [150], sont obtenus en [A10]. Rappelons que nos estimations d'erreur a posteriori permettent de distinguer et estimer séparément les différentes composantes d'erreur, en particulier la composante d'erreur correspondante à l'erreur de discrétisation (composante substantielle, donnée par le schéma numérique choisi et par la taille locale du maillage) et la composante d'erreur correspondante à l'erreur algébrique (composante subsidiaire, donnée par les itérations du solveur algébrique). Or, il est clair que l'erreur algébrique devient de plus en plus petite au fur et à mesure des itérations du solveur algébrique, alors que l'erreur de discrétisation stagne. En nous basant sur le point **iii)** du paragraphe 1.1.2, nous suggérons d'arrêter le solveur linéaire au moment où l'erreur algébrique n'affecte plus de façon significative l'erreur totale, c'est-à-dire quand l'erreur algébrique devient plus petite que celle de discrétisation. Ceci peut entraîner des économies de calcul importantes car un nombre élevé d'itérations du solveur algébrique linéaire peut être épargné. Nous discutons cette technique au paragraphe 3.1.

Critères d'arrêt pour des solveurs non linéaires

En utilisant des techniques similaires, des critères d'arrêt pour des solveurs non linéaires (par exemple la méthode de Newton ou la méthode du point fixe) sont dérivés en [A5], en développant les idées de Han [95] ou Chaillou et Suri [61, 62]. Une stratégie adaptative qui raffine le maillage du calcul aux endroits où l'erreur est grande et qui simultanément arrête le solveur non linéaire dès que possible est décrite au paragraphe 3.2.

Equilibrage des erreurs dans les sous-domaines et sur les interfaces dans des discrétisations par des joints

Dans [B3], on développe un algorithme adaptatif sur la base des estimations d'erreur a posteriori développées dans cette référence et suivant Wheeler et Yotov [175]. Cet algorithme équilibre les erreurs dans les sous-domaines et les erreurs dans les joints, de telle sorte qu'un calcul efficace puisse être fait afin d'obtenir une précision donnée. Nous présentons cet algorithme au paragraphe 3.3.

Une discrétisation adaptative d'un problème instationnaire de convection–diffusion–réaction permettant d'obtenir une précision donnée

Les estimations d'erreur a posteriori de [A7, A9] peuvent être divisées en deux parties correspondant à l'erreur en espace et à l'erreur en temps. Une telle approche a été déjà proposée, par exemple, dans Picasso [133], Verfürth [165], or Bergam et al. [38], mais le résultat principal ici est que le rapport entre les erreurs spatiales et temporales n'est pas influencé par une quelconque constante inconnue. Un algorithme adaptatif, permettant d'équilibrer ces deux composantes d'erreur substantielles, a été développé en [A9] pour l'équation de convection–diffusion–réaction instationnaire linéaire. Il est présenté au paragraphe 3.4, accompagné de quelques résultats numériques.

Une discrétisation adaptative d'un système instationnaire non linéaire couplé permettant d'obtenir une précision donnée

Enfin, un algorithme pour arrêter les solveurs algébriques et non linéaires quand les erreurs correspondantes n'affectent plus l'erreur totale et pour équilibrer les erreurs en espace et en temps, développé sur la base des estimations d'erreur a posteriori de [B4], est présenté au paragraphe 3.5. Il permet d'obtenir un calcul efficace et le contrôle de l'erreur au sens du paragraphe 1.1 pour le problème d'écoulement diphasique.

1.3.3 Implémentations, relations entre différentes méthodes numériques et post-traitement local

Le dernier thème de mes recherches après ma thèse de doctorat a été les implémentations peu coûteuses, les relations entre différentes méthodes numériques et le post-traitement local, cf. l'introduction du paragraphe 1.1.3. Mes contributions sur ce thème se trouvent dans les articles [A2, A8], les prépublications [B1, B5] et dans tous les travaux sur l'analyse a posteriori. Le but ici est de réaliser des implémentations peu coûteuses, de développer des cadres unifiés, d'améliorer les approximations par un post-traitement local et de présenter des analyses a priori non traditionnelles. Ces contributions font le sujet du chapitre 4.

Implémentations peu coûteuses et relations entre différentes méthodes numériques

La publication [B5] est une suite de l'article [170] qui fait partie de ma thèse de doctorat. Cet article donne un cadre pour des éliminations locales des inconnues du flux pour la méthode des éléments finis mixtes de plus bas degré ; par conséquent, ces méthodes peuvent être écrites avec une inconnue par maille uniquement, à la place d'une inconnue par élément et une inconnue par arête. Le but triple de [B5] est de présenter un cadre unifié, embrassant en particulier les résultats précédents de [170] et de Younès et al. [179], Chavent et al. [63] et Younès et al. [178], de montrer la proximité de la méthode des éléments finis mixtes et des différentes méthodes de type volumes finis et d'obtenir une implémentation peu coûteuse de la méthode des éléments finis mixtes répondant aux exigences en termes de coût de calcul réduit. Nous donnons plus de détails au paragraphe 4.1.1.

L'analyse de convergence d'une discrétisation d'une équation parabolique dégénérée de convection–diffusion–réaction par un schéma combinant les éléments finis affines par morceaux et les volumes finis centrés par maille sur des maillages non coïncidants est le sujet de [A8]. Cette analyse repose sur la proximité/équivalence de ces deux méthodes. Cet article est une suite de l'article [91] qui fait partie de ma thèse de doctorat et se fonde sur les résultats de Eymard et al. [87, 88, 90] ; ses résultats principaux sont décrits au paragraphe 4.1.2.

Améliorations des solutions approchées par un post-traitement local

La méthode des volumes finis centrés par maille donne des approximations constantes par morceaux uniquement. Ceci peut se révéler insuffisant dans beaucoup de cas. Nous introduisons dans [A12] une approximation localement post-traitée, fournissant une approximation parabolique par morceaux. Ce post-traitement constitue en fait la base des estimations d'erreur a posteriori de [A12]. Nous décrivons en détails ce post-traitement dans le paragraphe 4.2.1 et présentons un résultat de [A12] qui donne une estimation d'erreur a priori pour ce post-traitement sous la condition d'une régularité suffisante de la solution faible et un résultat de convergence sous une régularité minimale de la solution faible.

La méthode des éléments finis mixtes est ordinairement analysée dans le cadre de la formulation duale mixte, reposant sur la condition inf–sup de Babuška [20]–Brezzi [46]. Nous présentons au paragraphe 4.2.2 une nouvelle analyse a priori de la méthode des éléments finis mixtes, reposant sur un post-traitement local, la formulation faible primale et l'inégalité de Friedrichs discrète. Ce résultat était démontré en [A14] ; le post-traitement local est celui de [A11, Section 4.1], Arnold et Brezzi [19] et Arbogast et Chen [13]. En particulier, la condition inf–sup uniforme discrète peut être entièrement contournée et les deux analyses a priori et a posteriori peuvent être faites dans un cadre unifié.

Nous avons proposé dans [A1] une méthode d'éléments finis pour la discrétisation du contact entre deux membranes. La méthode proposée dans cette référence utilise néanmoins un nombre relativement élevé d'inconnues. Elle introduit, en particulier, une inconnue discrète fournissant l'approximation de l'action d'une membrane sur l'autre. L'approche de [A2] et de [B1] présente des formulations équivalentes avec des inconnues réduites aux approximations des positions des deux membranes seulement ; l'action d'une membrane sur l'autre est ensuite obtenue par un post-traitement local. Une estimation d'erreur a priori pour cette approximation post-traitée localement est aussi démontrée. Nous présentons les détails au paragraphe 4.2.3.

Dans tous les travaux mentionnés dans la partie sur l'analyse d'erreur a posteriori pour les méthodes non conformes localement conservatives du paragraphe 1.3.1 apparaît la notion d'une reconstruction du potentiel. Une telle reconstruction présente un intérêt en soi. Les méthodes en question donnent un potentiel discontinu et la présente reconstruction peut être utilisée à sa place. Nous présentons cette idée générale au paragraphe 4.2.4. De façon similaire, dans tous les travaux mentionnés dans la partie sur l'analyse d'erreur a posteriori pour les méthodes des éléments finis conformes ou de Galerkin discontinu du paragraphe 1.3.1 apparaît une notion d'une reconstruction du flux localement conservative. Cette reconstruction présente encore un intérêt en soi et nous la présentons au paragraphe 4.2.5.

Chapitre 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

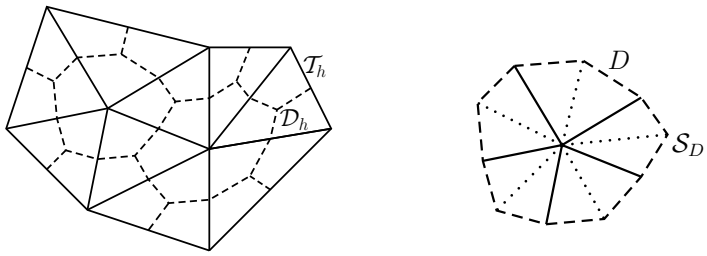

Figure 2.1: Original simplicial mesh $\mathcal{T}_h$ and an associated dual mesh $\mathcal{D}_h$ (left) and the fine simplicial mesh $\mathcal{S}_D := \mathcal{S}_h|_D$ of a dual volume $D \in \mathcal{D}_h$ (right)

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 $\mathbf{t}_h \in \mathbf{H}(\mathrm{div}, \Omega)$ 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

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

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,

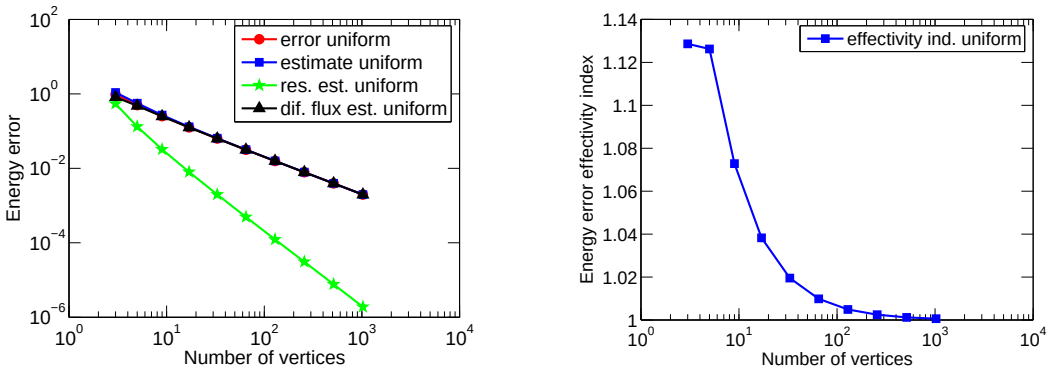

Figure 2.2: Estimated and actual energy error (left) and the corresponding effectivity index (right), vertex-centered finite volume method, problem (2.1a)–(2.1b) with a smooth solution in one space dimension

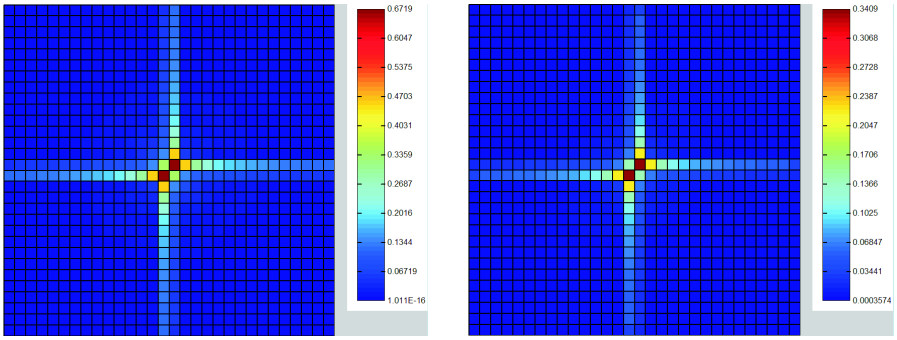

Figure 2.3: Estimated (left) and actual (right) energy error distribution, harmonic-weighted vertex-centered finite volume method, interface problem (2.1a)–(2.1b) with contrast 5 in the diffusion coefficient

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

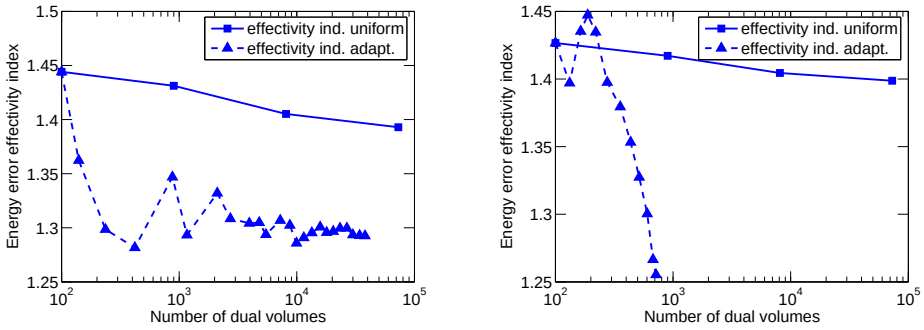

Figure 2.4: Energy error effectivity indices, harmonic-weighted vertex-centered finite volume method, interface problem (2.1a)–(2.1b) with contrast 5 (left) and 100 (right) in the diffusion coefficient

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

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

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

$$m_{K,\mathbf{S}} := C_{\mathrm{P},K}^{\frac{1}{2}} \frac{h_K}{c_{\mathbf{S},K}^{\frac{1}{2}}}.$$

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].

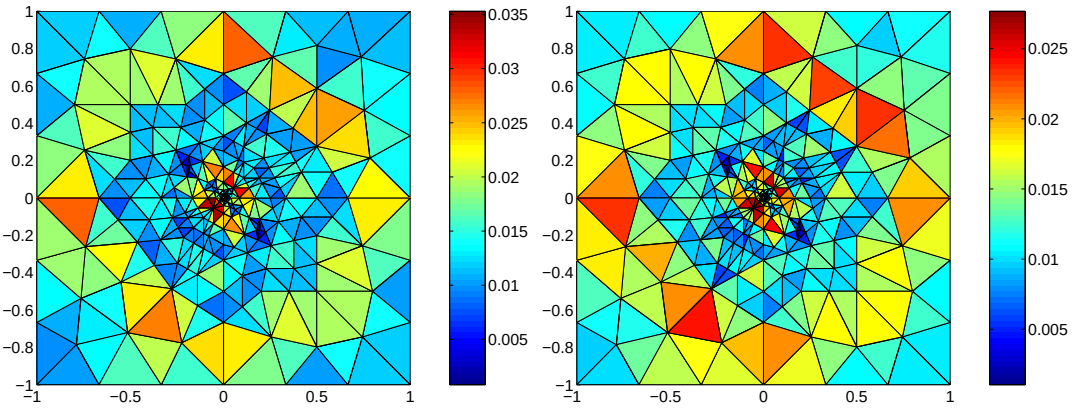

Figure 2.5: Estimated (left) and actual (right) energy error distribution, cell-centered finite volume method, interface problem (2.1a)–(2.1b) with contrast 5 in the diffusion coefficient

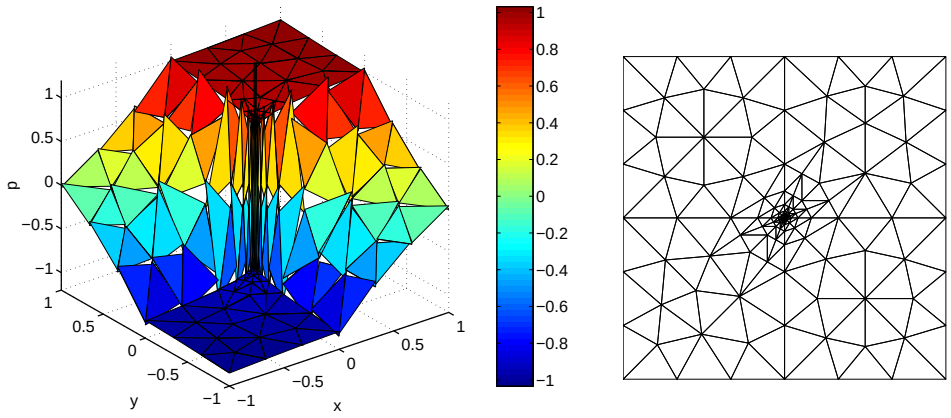

Figure 2.6: Approximate solution and the corresponding adaptively refined mesh, cell-centered finite volume method, interface problem (2.1a)–(2.1b) with contrast 100 in the diffusion coefficient

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

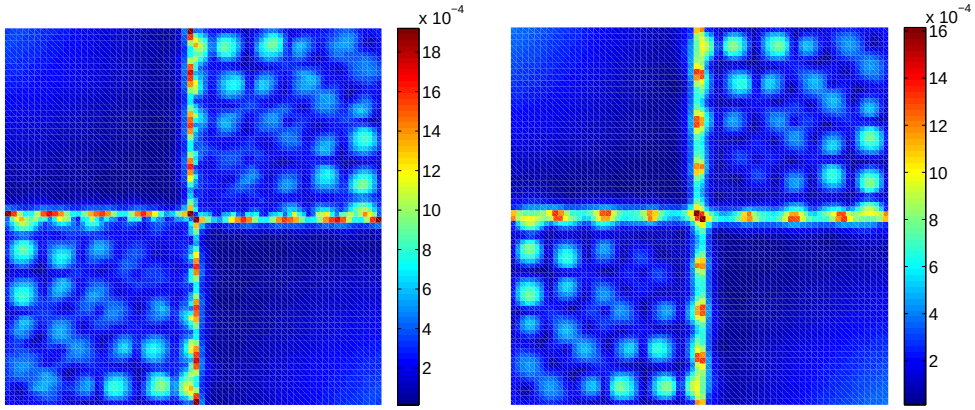

Figure 2.7: Estimated (left) and actual (right) flux error distribution on a nonmatching mesh with mortars, mortar mixed finite element method, problem (2.1a)–(2.1b)

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

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

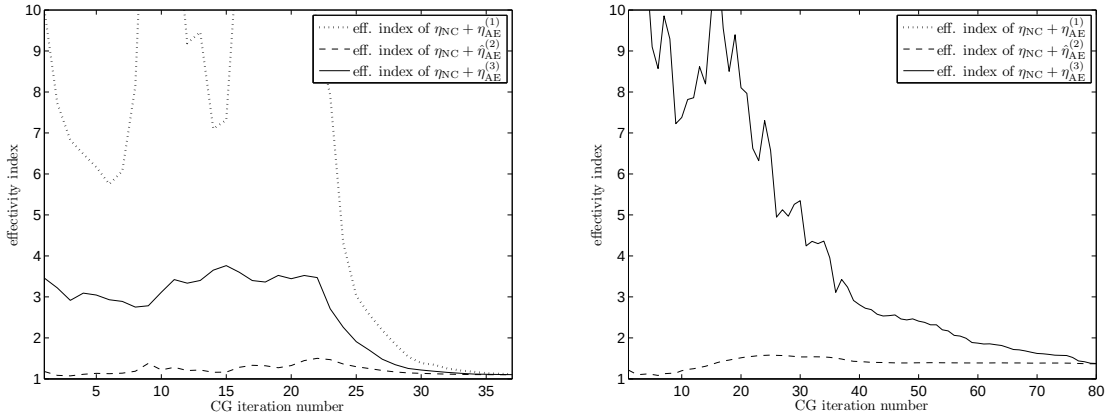

Figure 2.8: Effectivity indices for a posteriori error estimates including the algebraic error and the different algebraic estimators; problem (2.1a)–(2.1b) with a smooth solution (left) and with a contrast 100 in the diffusion coefficient (right)

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

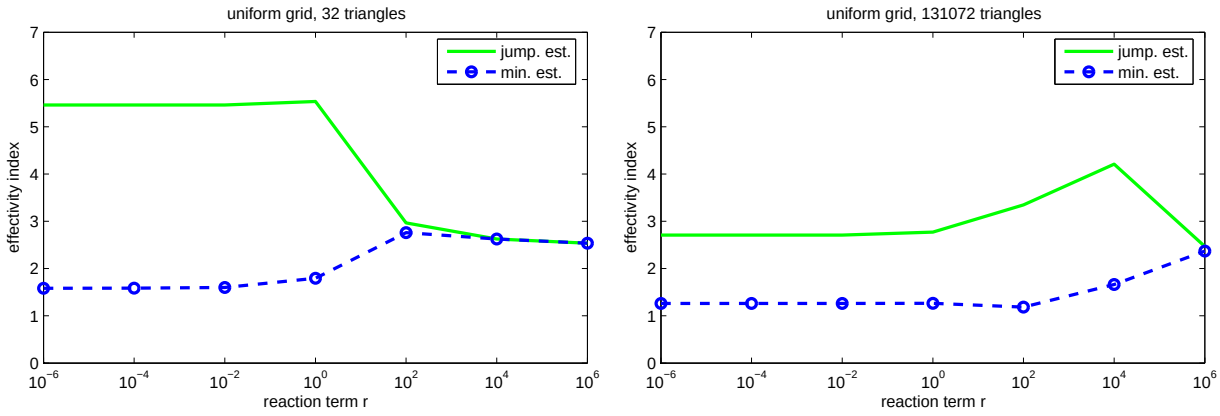

Figure 2.9: Effectivity indices in dependence on the reaction coefficient r of problem (2.28a)–(2.28b) for two different (uniformly refined) meshes, vertex-centered finite volume method

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

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

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*

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

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

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

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

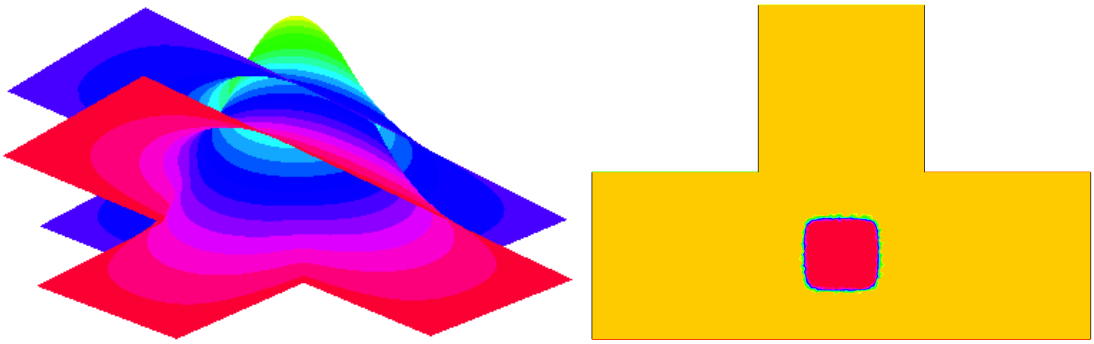

Figure 2.10: The displacements (left) and the action (right) for an adaptive discretization of the contact between membranes (2.40a)–(2.40e)

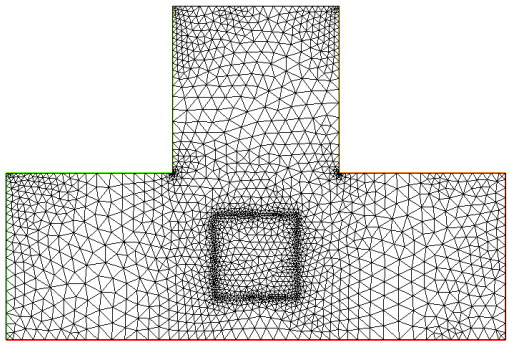

Figure 2.11: Adaptively refined mesh for the contact between membranes (2.40a)–(2.40e)

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

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

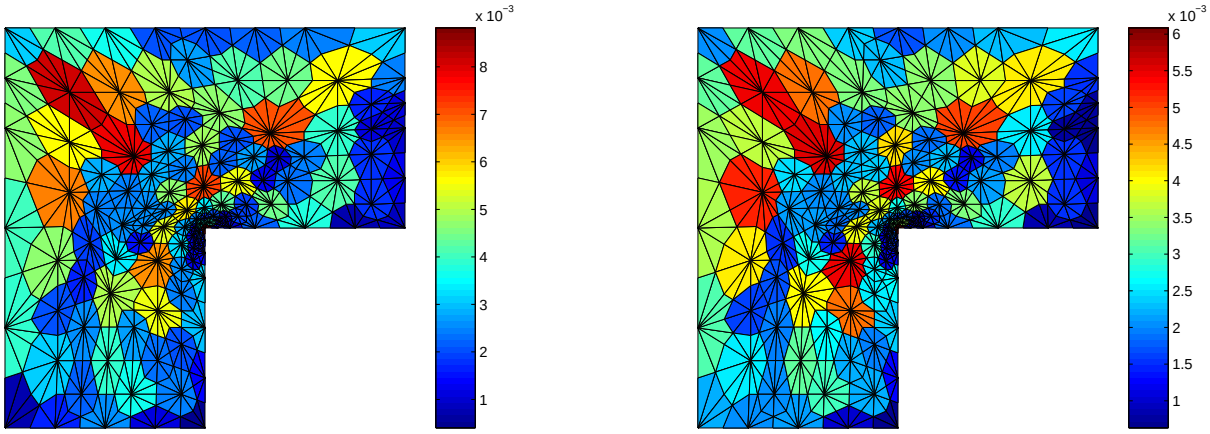

Figure 2.12: Estimated (left) and actual (right) error distribution; problem (2.41a)–(2.41b) with a singular solution, early stopped nonlinear solver

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

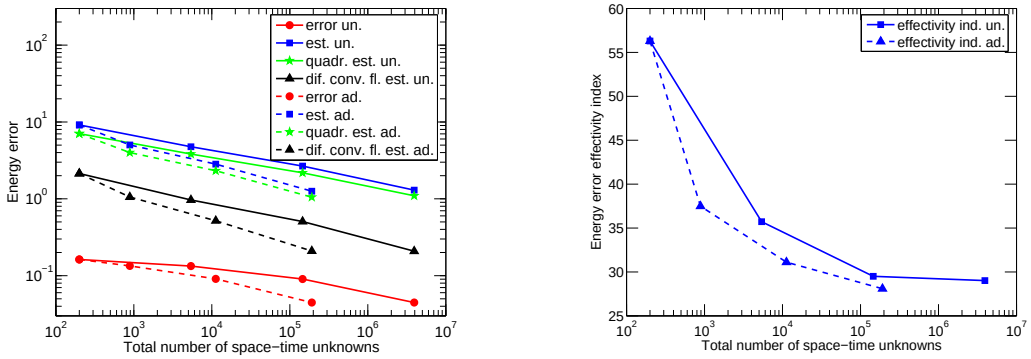

Figure 2.13: Estimated and actual energy error (left) and the corresponding effectivity index (right), combined finite volume–finite element method, instationary convection–diffusion–reaction problem

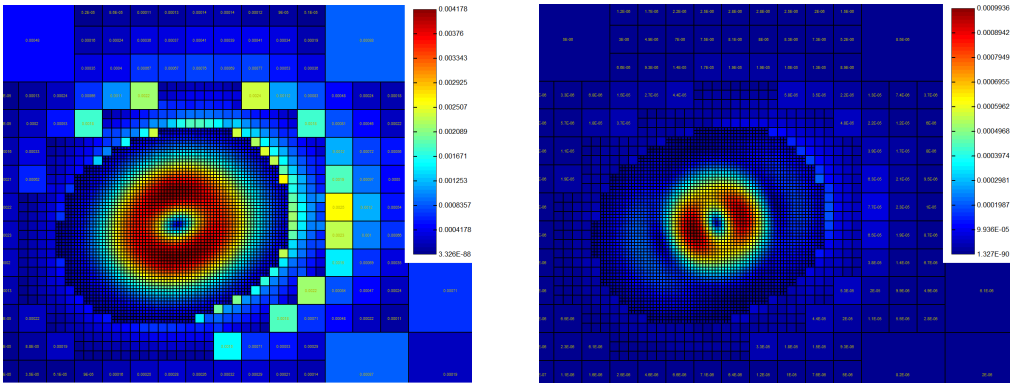

Figure 2.14: Estimated (left) and actual (right) energy error distribution, combined finite volume–finite element method, instationary convection–diffusion–reaction problem

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*

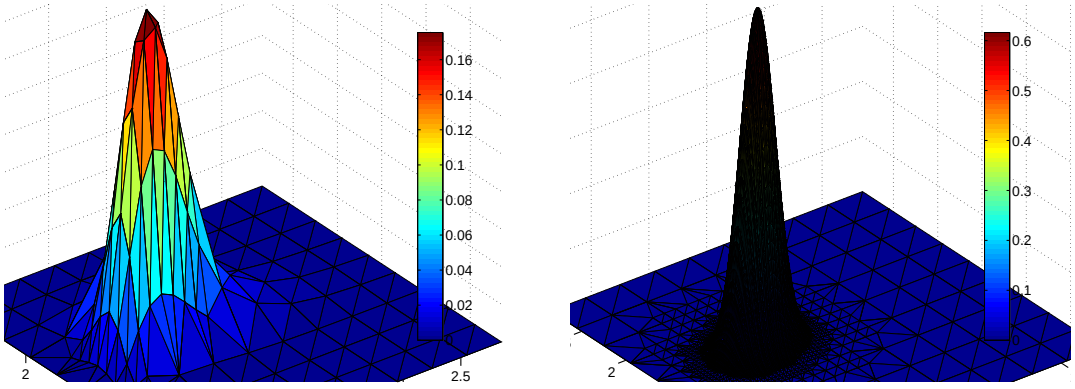

Figure 2.15: Examples of simulated plumes based on space-time adaptivity, two (left) and four (right) levels of refinement maximum, combined finite volume–finite element method, instationary convection–diffusion–reaction problem

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

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

Here $|||\cdot,\cdot|||$ stands for a dual norm similar to that of (2.44) and $\eta_{\mathrm{R},K,\alpha}^n$, $\eta_{\mathrm{DF},K,\alpha}^n$, and $\eta_{\mathrm{NC},K,\alpha}^n$ 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.

Chapitre 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

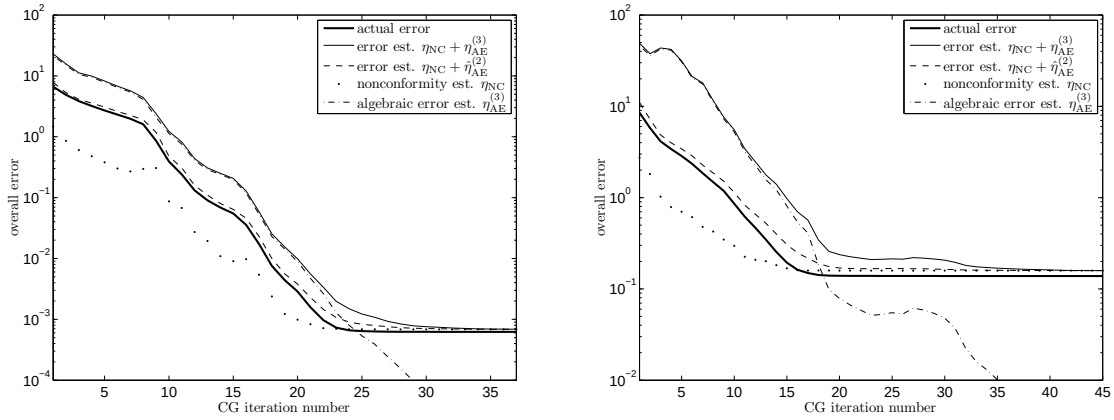

Figure 3.1: Energy error, overall estimators, and the algebraic and discretization estimators as a function of the number of iterations of the conjugate gradients iterative solver; problem (2.1a)–(2.1b) with a smooth solution (left) and with a contrast 100 in the diffusion coefficient (right)

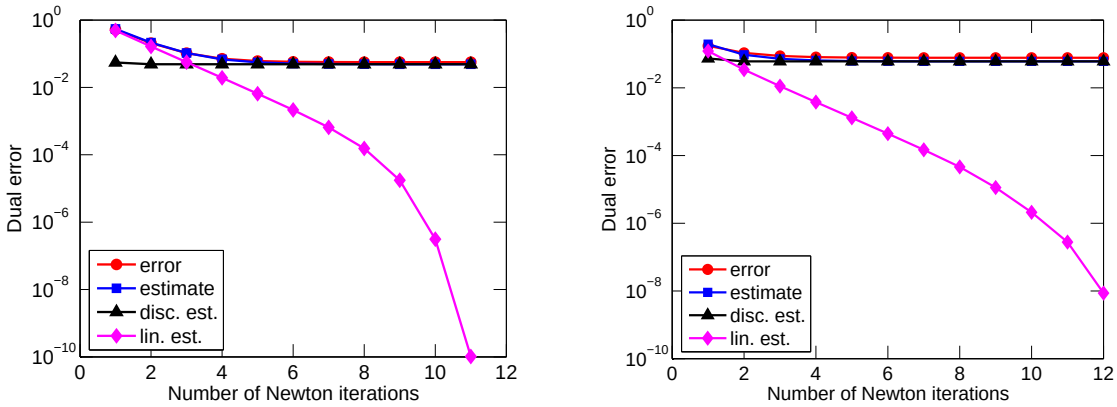

Figure 3.2: Dual error, overall estimator, and the linearization and discretization estimators as a function of the number of iterations of the Newton iterative solver; problem (2.41a)–(2.41b) with $q = 10$ (left) and $q = 50$ (right)

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

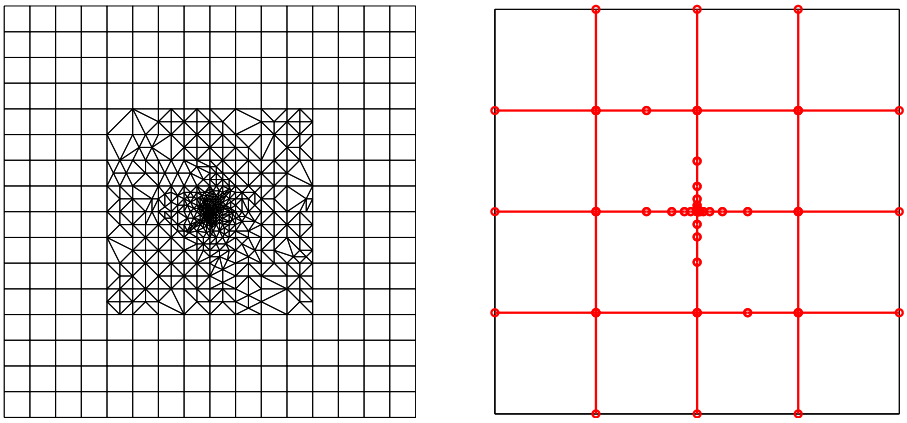

Figure 3.3: Adaptive subdomain (left) and mortar (right) meshes, mortar-coupled discontinuous Galerkin–mixed finite element method, problem (2.1a)–(2.1b)

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.

Chapitre 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].

Chapitre 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.

Appendice 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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ESTIMATIONS D'ERREUR A POSTERIORI, CRITERES D'ARRET ET IMPLEMENTATIONS PEU COUTEUSES

pour contrôle d'erreur et efficacité dans des simulations numériques

Résumé

Cette habilitation porte sur des algorithmes numériques pour la discrétisation des équations elliptiques et paraboliques de convection–diffusion–réaction linéaires et non linéaires, des équations de Stokes et d'une inégalité variationnelle modèle. L'attention principale est sur le développement d'algorithmes qui permettent d'atteindre une précision donnée par l'utilisateur. Le calcul devrait en plus être efficace dans le sens où la quantité de travail nécessaire est la plus petite possible.

Notre instrument de base sont les estimations d'erreur a posteriori. Nous les développons pour plusieurs méthodes numériques classiques, volumes finis, éléments finis, éléments finis mixtes ou la méthode de Galerkin discontinue. Nous proposons plusieurs cadres unifiés, embrassant toutes ces méthodes. Nous nous concentrons sur des estimations optimales, à savoir des estimations : i) garanties dans le sens où une borne supérieure d'erreur entre la solution exacte inconnue et la solution approchée connue, entièrement calculable, est donnée ; ii) efficaces localement dans le sens où elles donnent une borne inférieure locale à l'erreur ; iii) asymptotiquement exactes, c'est-à-dire telles que l'index d'efficacité (le rapport entre l'erreur estimée et l'erreur actuelle) tend vers 1 en augmentant le coût du calcul ; iv) robustes dans le sens où que les trois propriétés précédentes sont valables indépendamment des paramètres et de leur variation ; et v) pouvant être évaluées pour un coût négligeable.

Nos estimations permettent de distinguer, d'estimer séparément et de comparer les différentes composantes de l'erreur. On peut par la suite arrêter les différents algorithmes itératifs (solveurs itératifs linéaires, solveurs itératifs non linéaires) au moment où les erreurs subsidiaires correspondantes diminuent en deçà du niveau où elles n'affectent plus l'erreur totale. On peut aussi ajuster les paramètres du calcul (par exemple les maillages en espace ou les pas de temps) de telle sorte que les erreurs substantielles (l'erreur de discrétisation en espace, l'erreur de discrétisation en temps) soient distribuées de façon équilibrée et de grandeurs comparables. A l'aide d'une telle adaptativité, l'efficacité des simulations numériques et le contrôle de l'erreur peut être atteinte.

La dernière partie de cette habilitation est dédiée aux implémentations peu coûteuses et les relations entre différentes méthodes numériques, ce qui en particulier permet de développer des cadres unifiés. Nous montrons également comment obtenir des approximations améliorées par le post-traitement local et présentons des analyses a priori non traditionnelles.

Tous les articles de cette habilitation contiennent des résultats théoriques. Certains décrivent aussi des implémentations d'algorithmes adaptatifs dans des codes de calcul et la plupart sont étroitement liés aux applications telles que l'écoulement et transport de contaminants en milieu poreux, les écoulements diphasiques ou des problèmes de contact unilatéral.

Mots clés : problème de convection–diffusion–réaction du second degré, problème de Stokes, problème monotone non linéaire, problème parabolique dégénéré, inégalités variationnelles, méthode des volumes finis, méthode des éléments finis, méthode des éléments finis mixtes, méthode de Galerkin discontinue, maillages non coïncidants, multi-échelles, multi-numérique, technique des joints, existence et unicité, convergence, estimation d'erreur a priori, estimation d'erreur a posteriori, méthodes itératives pour des systèmes linéaires algébriques, linéarisation itérative, critères d'arrêt, équilibrage des composantes d'erreur, raffinement du maillage adaptatif, calcul efficace, contrôle de l'erreur, relations entre différentes méthodes, expressions locales des flux, post-traitement local, cadre unifié, robustesse, écoulement et transport de contaminants, écoulement diphasique, milieu poreux, contact unilatéral, membranes élastiques

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