Mathematisches Forschungsinstitut Oberwolfach

Report No. 29/2007

Adaptive Numerical Methods for PDEs

Organised by
Rolf Rannacher, Heidelberg
Endre Süli, Oxford
Rüdiger Verfürth, Bochum

June 10th – June 16th, 2007

Abstract. This collection contains the extended abstracts of the talks given at the Oberwolfach Conference on "Adaptive Numerical Methods for PDEs", June 10th - June 16th, 2007. These talks covered various aspects of a posteriori error estimation and mesh as well as model adaptation in solving partial differential equations. The topics ranged from the theoretical convergence analysis of self-adaptive methods, over the derivation of a posteriori error estimates for the finite element Galerkin discretization of various types of problems to the practical implementation and application of adaptive methods.

Mathematics Subject Classification (2000): 65xx, 65Mxx, 65Nxx, 73Vxx, 76Mxx.

Introduction by the Organisers

Multidimensional processes in sciences and engineering are usually formulated in terms of partial differential equations. With the incorporation of more and more complete physics these models become increasingly complex. Their accurate numerical simulation requires the use of efficient methods which exploit concepts of adaptivity in setting up the models and their discretization. Over the last two decades these approaches have been developed from simple model situations towards real-life applications, in most cases with striking success. The conference "Adaptive Numerical Methods for PDEs" had its focus on basic questions related to the rigorous mathematical understanding of these methods and to their practical use.

The use of automatic adaptivity has become common in the simulation of all kind of PDE models even in situations where a solid theoretical justification is lacking. Examples are the nonlinear Navier-Stokes equations in fluid mechanics, the nonlinear Lamé-Navier equations in large-strain elasticity, the Maxwell equations,

and combinations of these models in nonstationary fluid-structure interaction and magneto-hydrodynamics. Such approaches are usually based on *a posteriori* information in terms of local quantities such as approximate gradients or residuals obtained from the computed solution. The extension of quantitative mathematical analysis of adaptive methods to such complicated models is a challenging problem.

The existing methods of a posteriori error estimation and mesh adaptation are based on several heuristic technical assumptions. These are assumptions about the convergence of higher-order difference quotients, the relative "smallness" of linearization errors, "sharpnes" of stopping criteria of algebraic iterations, the "safe" control of error accumulation in long-time calculations, etc. These aspects are fundamental to adaptive methods and still need rigorous mathematical analysis for a better understanding of the underlying mechanisms.

Recently, several new directions of adaptivity have evolved, e.g., "spectral-adaptivity" in wavelet analysis, "hp-adaptivity" in high-order FE-methods, "anisotropic" refinement in the approximation of layers, adaptivity in the solution of "optimal control" problems, "model adaptivity" for example in spatial dimension reduction or the complexity reduction in diffusion models, and "multi-scale" adaptivity in problems with micro- and macro-scales reaching even towards adaptive turbulence modeling. The latter are the really "hot" topics in current Numerical Analysis research. The mathematical analysis of these approaches has to combine concepts of a posteriori error estimation with techniques from PDE theory. The talks given at this conference were concerned with the following subjects:

- Concepts of model adaptivity;
- Adaptive multi-scale analysis;
- Adaptivity in optimal control;
- Error control in iterative solution processes;
- Anisotropic mesh adaptation;
- Higher-order adaptive FE hp-methods;
- Error control of linearization and stabilization;
- Local "goal-oriented" versus global "norm-based" error estimation;
- Mathematical analysis of *a posteriori* error estimates;
- Convergence of adaptive algorithms.

Workshop: Adaptive Numerical Methods for PDEs

Table of Contents

Abstracts

Error estimation and adaptivity for inverse problems

Wolfgang Bangerth
(joint work with Amit Joshi)

Inverse problems are an important class of PDE-constrained optimization problems that attempt to reconstruct unknown material properties from measurements of how a system responds to a known external force. In their most general, nonlinear form they are usually posed as an optimization problem in which one wants to minimize the difference between actual measurements z and prediction measurements Mu, where u satisfies a partial differential equation $L(q)u = f$ in which the operator depends on a set q of a priori unknown parameters, and f is a known forcing term. M is an operator that extracts from the predicted response of the system, u, those aspects that are physically measured in the experiment. The problem to be solved can then be stated as follows (more general formulations for nonlinear forward problems or more than one measurement can be found in [2]):

$$\min_{u,q} \frac{1}{2}\|Mu - z\|^2$$
$$\text{subject to } L(q)u = f.$$

A common approach for solving this is to introduce a Lagrangian

$$L(u, q, \lambda) = \frac{1}{2}\|Mu - z\|^2 + \langle L(q)u - f, \lambda\rangle$$

and seeking the solution of the orginal problem as a stationary point of this Lagrangian. This leads to a set of coupled, nonlinear partial differential equations that have to be solved simultaneously.

By choosing appropriate discrete subspaces for the variables u, q, λ, this problem can be solved by applying a Newton method to a discrete version of the optimality condition, or better even to apply Newton's method to the optimality condition and separately discretizing each Newton step using the finite element method on a sequence of meshes that become finer as Newton iterations proceed. However, given the size of practical inverse problems, which often ranges into millions of unknowns, the actual solution of realistic problems is computationally very expensive. Efficient adaptive finite element methods based on error estimates are therefore important tools to allow the solution of such problems.

Deriving error estimates for inverse problems is complicated by the fact that they are typically ill-posed, i.e. there is continuous relationship between data and solution. Consequently, the typical way of using stability estimates of solutions (for energy estimates) or solutions to dual problems (in the case of goal-oriented estimates) does not work: the stability constant is very large or infinite. This observation in itself is of only academic interest since it also prevents the problem from being solved at all, and forces us to introduce regularization terms into the objective function, i.e. to minimize $\frac{1}{2}\|Mu - z\|^2 + \beta\|q\|^2$, where the two norms

are appropriately chosen to make the problem well-posed. This regularized formulation is stable, and error estimates using stability estimates have been derived in the past. However, they are mostly useless for practical purposes: the stability constant is proportional to $\frac{1}{\beta}$, but one would like to choose β as small as possible since the original goal was to minimize the misfit $Mu - z$, not the regularization term. In practice, stability-based error estimates are therefore of little value and hopelessly overestimate the errors by orders of magnitude.

We therefore propose an alternative approach in which we numerically compute a dual solution as well, following the general methodology outlined in [4, 10, 3]. In this approach, called the dual-weighted residual (DWR) method, stability is not considered in the worst-case scenario as a constant, but as a sensitivity function obtained by linearizing the problem around the current solution. They are therefore much more accurate (with efficiency factors between 0.5 and 3 in some situations). Furthermore, if the goal functional happens to be the objective function of the optimization problem, then the dual solution turns out to be equal to the primal one, and no additional problem has to be solved. The evaluation of such error estimates is therefore no more expensive than that of more traditional estimates that weight a norm of the residual with a stability constant and appropriate powers of the local mesh size.

In the talk, we present the derivation of this approach as previously shown in [3, 1] as well as numerical results obtained for a variety of inverse problems. In particular, we will show results from an optical tomography application in biomedical imaging [7, 6, 8, 9, 2]. For these realistic inverse problems, the equations are often very lengthy and complicated, and actually implementing DWR error estimates becomes a challenge. We therefore extract the essential features of the DWR method, namely of weighing primal residuals with dual solutions and vice versa, and apply it to the problem at hand. Examples will illustrate that this problem is not solvable at all using uniformly refined meshes within realistic time and memory requirements, but can be solved on workstations within clinically almost acceptable 10-20 minutes using adaptive finite element meshes derived through the DWR method.

References

[1] W. Bangerth. *Adaptive Finite Element Methods for the Identification of Distributed Parameters in Partial Differential Equations*. PhD thesis, University of Heidelberg, 2002.

[2] W. Bangerth. A framework for the adaptive finite element solution of large inverse problems. Technical Report ISC-2007-03-MATH, Institute for Scientific Computation, Texas A&M University, 2007.

[3] W. Bangerth and R. Rannacher. *Adaptive Finite Element Methods for Differential Equations*. Birkhäuser Verlag, 2003.

[4] R. Becker and R. Rannacher. Weighted a posteriori error control in FE methods. In et al. H. G. Bock, editor, *ENUMATH 95*, pages 621–637, Paris, September 1998. World Scientific Publ., Singapure. in [5].

[5] H. G. Bock, F. Brezzi, R. Glowinsky, G. Kanschat, Y. A. Kuznetsov, J. Périaux, and R. Rannacher, editors. *ENUMATH 97, Proceedings of the 2nd European Conference on Numerical Mathematics and Advanced Applications*, Singapore, 1998. World Scientific.

[6] A. Joshi, W. Bangerth, K. Hwang, J. C. Rasmussen, and E. M. Sevick-Muraca. Fully adaptive fem based fluorescence optical tomography from time-dependent measurements with area illumination and detection. *Med. Phys.*, 33(5):1299–1310, 2006.
[7] A. Joshi, W. Bangerth, K. Hwang, J. C. Rasmussen, and E. M. Sevick-Muraca. Plane wave fluorescence tomography with adaptive finite elements. *Optics Letters*, 31:193–195, 2006.
[8] A. Joshi, W. Bangerth, and E. M. Sevick-Muraca. Adaptive finite element modeling of optical fluorescence-enhanced tomography. *Optics Express*, 12(22):5402–5417, November 2004.
[9] A. Joshi, W. Bangerth, and E. M. Sevick-Muraca. Non-contact fluorescence optical tomography with scanning patterned illumination. *Optics Express*, 14(14):6516–6534, 2006.
[10] R. Rannacher. The dual-weighted-residual method for error control and mesh adaptation in finite element methods. In J.R. Whiteman, editor, *Proc. MAFELAP 1999*, pages 97–116. Elsevier, Amsterdam, 2000.

Adaptive Methods and Near-Best Tree Approximation

Peter Binev

Large scale problems require fast and efficient ways of processing. Computational tractability can often be guaranteed only by methods that are nonlinear in nature and at the same time support efficient data structures. Tree approximation is a paradigm that takes up both issues. It provides an efficient way of storing the coefficients in wavelet expansions while essentially preserving the optimal rate of the N-term approximation. It is also a natural way of representing the partitions generated by adaptive solvers for PDEs.

Previously known results (see [3]) provide optimality of asymptotic rates over a whole class of functions. The corresponding algorithms which realize such an approximation have only theoretical significance. The question is: *Can we achieve instance optimality in the sense of recovering the best N-term rate for each individual function?* To answer this question we outline a specific approximation scheme which achieves just that.

We represent the adaptively generated partitions as proper subtrees of an infinite *master* tree $\mathcal{T}$. The master tree $\mathcal{T}$ is fixed and corresponds to a particular subdivision procedure used in the adaptive process which produces the partitions. Here "proper" means that T corresponds to a partition, namely that it contains the subtree T_0 which corresponds to the initial partition and if a node Δ of T is not a leaf, then the set $\mathcal{C}(\Delta)$ of all its children is contained in T. We assume that at each node Δ of $\mathcal{T}$ it is given an error $e(\Delta)$ which can be calculated using a fixed number of operations. The total error $E(T)$ of the partition corresponding to the tree T can be calculated as the sum of the errors at the leaves $\mathcal{L}(T)$ of T

$$E(T) := \sum_{\Delta\in\mathcal{L}(T)} e(\Delta) \ .$$

Often in practice it is impossible to calculate the actual error and one has to use some local quantities to represents the local errors $e(\Delta)$. A necessary condition to these quantities is the *subadditivity* property

$$e(\Delta) \geq \sum_{\Delta'\in\mathcal{C}(\Delta)} e(\Delta') \ . \tag{1}$$

Sometimes it is desirable to relax the above condition by requiring that there exists a constant $C_0 > 0$ such that

$$e(\Delta) \geq C_0 \sum_{\Delta' \in \mathcal{L}(T_\Delta)} e(\Delta') \tag{2}$$

for every subtree $T_\Delta \subset \mathcal{T}$ rooted at Δ.

Let N_0 be the number of leaves of the initial tree T_0 and let $N(T)$ be the number of subdivisions performed consecutively to T_0 in order to receive T. Evidently, $N(T) = \#(T) - \#(\mathcal{L}(T)) - \#(T_0) + N_0$ is the number of new internal nodes of T. Using this notation we can introduce the *best n-term tree approximation* by

$$\sigma_n = \sigma_n(\mathcal{T}) := \min_{T: N(T) \leq n} E(T)$$

and ask the question whether there exists an $\mathcal{O}(n)$ algorithm that finds a tree which complexity and error are within (small) multiplicative constants from the ones of σ_n. The answer to this question is given in [1]. The algorithm proposed there defines *modified* errors by the following rules

$$\tilde{e}(\Delta) := e(\Delta) \text{ for } \Delta \in T_0 \qquad \text{and} \qquad \tilde{e}(\Delta) := \frac{\sum_{\Delta'' \in \mathcal{C}(\Delta')} e(\Delta'')}{e(\Delta') + \tilde{e}(\Delta')} \text{ for } \Delta \in \mathcal{C}(\Delta') \,. \tag{3}$$

Then the tree T is received adaptively from T_0 by subdividing at each step the current leaf node Δ with the largest modified error. (Alternatively, to avoid sorting we can group the modified errors into bins based on their values and choose one which is within a small multiplicative constant from the largest.) Here we shall refer to the above algorithm as *old tree algorithm*. The main result for it is the following

Theorem 1 [1] *Let the number of the children at each node of $\mathcal{T}$ be limited by a constant K. Then there exists a constant $C > 0$ such that at each step the output tree T of the* old tree algorithm *satisfies*

$$E(T) \leq C\sigma_n(\mathcal{T})$$

whenever $n \leq N(T)/(2K+2)$. To create T the algorithm uses less than $C(N(T)+N_0)$ arithmetic operations and computations of e.

The constant C in the above theorem is given explicitly and depends on K and C_0. It is interesting to know whether this constant can be arbitrarily close to 1. In the case $C_0 = 1$ we have the following result

Theorem 2 *If $\mathcal{T}$ is a binary tree (i.e. $K = 2$) and the errors $e(\Delta)$ in it satisfy the subadditivity condition (1), then the output tree T of the* old tree algorithm *satisfies*

$$E(T) \le \left(1 + \frac{2(n + N_0)}{N(T) - n + 1}\right)\ \sigma_n(\mathcal{T})$$

whenever $n \le N(T)$.

Using the above theorem the following variant of Corollary 5.4 from [1] can be derived

Corollary 3 *Let $\mathcal{T}$ be a binary tree and the errors $e(\Delta)$ satisfy the subadditivity condition (1). If the tree T_μ is the first tree from the sequence of outputs of* old tree algorithm *that satisfies $E(T_\mu) \le \mu$, then*

$$N(T_\mu) \le \frac{2(1 + c_1)}{1 - c_1}\ N(T)$$

for $0 < c_1 < 1$ and any proper subtree T of $\mathcal{T}$ with $E(T) \le c_1\mu$.

The performance of old tree algorithm can be improved by replacing the definition of the modified errors in (3) with the following one

$$(4)\ \ \tilde{e}(\Delta) := e(\Delta) \text{ for } \Delta \in T_0 \quad \text{and} \quad \tilde{e}(\Delta) := \left(\frac{1}{e(\Delta)} + \frac{1}{\tilde{e}(\Delta')}\right)^{-1} \text{ for } \Delta \in \mathcal{C}(\Delta').$$

We shall refer to that algorithm as *new tree algorithm*. The following theorem shows that the constant C no longer depends on K. However, the complexity of the algorithm still depends on K via the total number of nodes in T which can be estimated by $K\,N(T)$.

Theorem 4 *Let the errors $e(\Delta)$ in $\mathcal{T}$ satisfy the subadditivity condition (1). Then at each step of the* new tree algorithm *the output tree T satisfies*

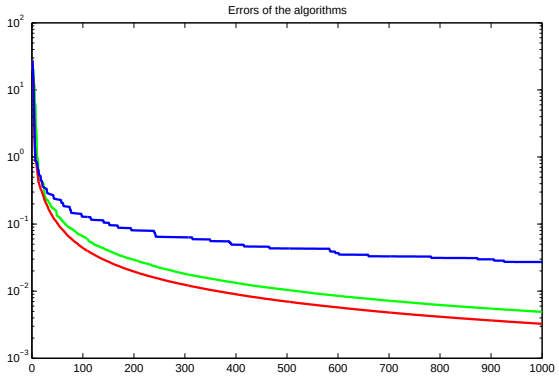
$$E(T) \le \left(1 + \frac{n + \min\{n, N_0\}}{N(T) - n + 1}\right)\ \sigma_n(\mathcal{T})$$

whenever $n \le N(T)$.

To illustrate the fact that the greedy approach cannot give a near-best performance, we consider a simple example of finding the best L_2-approximation via piecewise constants on dyadic partitions for the function $f(x) = (\sqrt{x}\ln(x/1.02))$. For this example the performance of the greedy algorithm is worse by a logarithmic factor.

In the figure the errors of the described algorithms for the first 1000 iterations are presented: the greedy algorithm is the top graph (in blue), in the middle (in green) is the algorithm proposed in [1], while the best performance has the new tree algorithm represented by the bottom graph (in red).

We conclude with indicating some consequences of the results about near-best tree approximation. In particular, we compare the adaptive schemes for solving elliptic PDEs and consider the conditions needed to establish instance optimality of the solution. The overwhelming majority of these methods is based on local



error estimates which sum gives reliable information about the total error. The method is often described with the iterated scheme

$$\text{MARK} \rightarrow \text{REFINE} \rightarrow \text{SOLVE} \quad \hookleftarrow . \tag{5}$$

The most popular among the marking strategies is the *bulk chasing* [4]. However, these strategies apply the greedy approach in choosing the elements for subdivision which does not give much hope for instance optimality results. A convergence result together with an error reduction property was first derived in [5] for a variant of (5) with the bulk chasing strategy in the case of Poison equation and the newest vertex bisection subdivision procedure. Optimal convergence rates were first received in [2] based on the error reduction property from [5]. The paper [2] establishes the theoretical justification of all the steps in the algorithm. It also shows that the sparsity of the solution is necessary for the optimality of the algorithm and to secure it adds the COARSENING step to (5). The inclusion of this step gives the freedom to use any error reduction procedure (and in particular the one consisting of several loops of (5)). Then, the obtained approximation should be checked for sparsity and a certain action should be taken so that the approximate solution will stay sparse. In general, the idea of the algorithm can be summarized in the scheme

$$\text{ERROR REDUCTION} \rightarrow \text{SPARSITY ADJUSTMENT} \quad \hookleftarrow . \tag{6}$$

This approach is able to give instance optimality results in the following sense: given the differential equation $Lu = f$, if the differential operator L and the function f are approximated with tolerance $\varepsilon > 0$, then the approximate solution is near-best or the error is below ε. In comparison, it was shown in [6] that the optimal rates of convergence can be achieved using a variant of the bulk chasing method with carefully selected (small) bulk constant. In some sense this method combines the steps in (6). However, its optimality is only in terms of asymptotic behavior. Thus, the performance can be very poor in terms of an individual functions and a fixed number of degrees of freedom. Note that in the example for tree approximation the greedy approach also has optimal rates, but the constants are growing as $\log n$.

In conclusion, the tools provided by near-best adaptive tree approximation can be used to obtain methods fitting the scheme (6) which can give instance optimality results for a wide range of problems.

References

[1] P. Binev, and R. DeVore, *Fast Computation in Adaptive Tree Approximation*, Numer. Math. **97** (2004), 193–217.

[2] P. Binev, W. Dahmen, and R. DeVore, *Adaptive Finite Element Methods with Convergence Rates* , Numer. Math. **97** (2004), 219–268.

[3] A. Cohen, W. Dahmen, I. Daubechies, R. DeVore, *Tree approximation and optimal encoding*, Appl. Comp. Harm. Anal. **11** (2001), 192–226.

[4] W. Dörfler, *A convergent adaptive algorithm for Poisson's equation*, SIAM J. Numer. Anal. **33** (1996), 1106–1124.

[5] P. Morin, R. Nochetto, and K. Siebert, *Data Oscillation and Convergence of Adaptive FEM*, SIAM J. Numer. Anal. **38** (2000), 466–488.

[6] R. Stevenson, *Optimality of a standard adaptive finite element method*, Found. Comput. Math. **7** (2007), 245–269.

Unified a posteriori error analysis of nonstandard finite element methods

Carsten Carstensen

General strategies are discussed to derive a posteriori error estimates for conforming, mixed, and nonconforming finite element methods in energy norms which also cover discontinuous Galerkin schemes or Mortar finite elements for second order elliptic problems. The unifying approach provides reliable error estimates which can be shown to be efficient as well. The goal is to prove that *all* nonstandard schemes allow for (some) a posteriori error control, there is no finite element method known to the author where there is no error control.

Surprisingly, there remains one type of residuals R for different problems, such as, the Laplace problem, the Stokes problem, and Navier-Lamé problem, with conforming, nonconforming, and mixed finite element method. One key observation is that

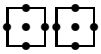
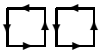
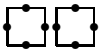
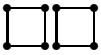
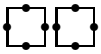
$$\mathrm{Res}(v) := \int_\Omega g \cdot v dx + \int_{\cup\mathcal{E}} g_\mathcal{E} \cdot v ds \quad \text{for } v \in V := H^1_0(\Omega;\mathbb{R}^m)$$

is the same (or at least very similar) for all those schemes. Based on some Galerkin property, the kernel of the residual $\mathrm{Res} \in V^* = H^{-1}(\Omega;\mathbb{R}^m)$ includes a space V_h^{NC}. This space V_h^{NC} can be mapped onto some first- order conforming finite element space $V_h^C \subset V := H^1_0(\Omega;\mathbb{R}^m)$. In all cases the author is aware of, there exists some operator $\Pi : V_h^C \to V_h^{NC}$ with some elementwise properties such that a unifying analysis is possible.

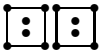
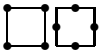
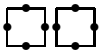
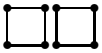
Some nonconforming elements [1,2,3] for the Poisson problem, the Stokes problem, and linear elasticity in two dimensions are depicted in the following tables. The point is that the analysis simultaneously discusses all of those (and even more).

picture	name
	Crouzeix-Raviart
	Wilson
	Han
	NR (M)
	NR (A)
	CNR
	DSSY

NCFEM for Laplace

picture	name
	Crouzeix-Raviart
	Kouhia-Stenberg
	Han
	NR (M)
	NR (A)
	HMS
	CJY

NCFEM for Stokes

picture	name
	Brenner-Sung
	Kouhia-Stenberg
	Zhang
	Ming
	LLS
	HMS

NCFEM for Navier-Lamé

Particular application to discontinuous Galerkin methods from [4] are outlined.

The conclusion of this presentation is sparsity in the mathematical research of a posteriori error control. The reduction is to two parts. (a) Analyze the PDE in such a way that the error is equivalent to the dual norm of the residual $\| \operatorname{Res} \|_*$ and analyze $V_h \subset \ker \operatorname{Res}$. (b) Design general a posteriori error estimates for $\| \operatorname{Res} \|_*$ independently of the PDE.

The presentation summarises joint work with Jun Hu, Antonio Orlando, Max Jensen and T. Gudi.

References

[1] C. Carstensen, A unifying theory of a posteriori finite element error control, Numer.Math, 100 (2005),617–637.

[2] C. Carstensen, Jun Hu, A. Orlando, Framework for the a posteriori error analysis of nonconforming finite elements, Preprint (2005-11), Department of Mathematics, Humboldt University of Berlin (2005). SINUM (2007), in press.
[3] C. Carstensen and Jun Hu, A Unifying Theory of A Posteriori Error Control for Nonconforming Finite Element Methods, Preprint (2006-21), Department of Mathematics, Humboldt University of Berlin (2006), Numerische Mathematik (2007) in press.
[4] C. Carstensen, T. Gudi, M. Jensen, A Unifying Theory Of A Posteriori Error Control For Discontinuous Galerkin FEM, 2007 in preparation.

Pointwise estimators and pollution on polyhedral domains

Alan Demlow

Adaptive methods for controlling pointwise errors are desirable in many situations. In order to motivate our talk, we give two examples in the case of elliptic problems. First, mixing problems were studied in the recent Ph.D. thesis [6] of E. Svensson. The goal there was to track particle trajectories satisfying $\vec{x}(t) = \vec{u}(\vec{x})$, where $\vec{u}$ is the velocity field determined by the stationary Stokes equation. A "shadowing estimator" for $\vec{x}$ developed by Svensson requires bounds for $\|\nabla(\vec{u} - \vec{u}_h)\|_{L_\infty(\Omega)}$, where $\vec{u}_h$ is a finite element approximation to $\vec{u}$. If Ω here is a nonconvex polyhedral domain, then one must seek bounds for $\nabla(\vec{u} - \vec{u}_h)$ on some subset D of Ω not abutting reentrant corners. Another class of examples involves computations in which the goal output is a subset of the overall computational domain rather than some norm or functional of the solution. In the context of elliptic problems, one such problem is the determination of the location and volume of the region where the stresses in a material exceed a given threshold; cf. [4]. Note that in both of these examples, the information desired from the calculation is potentially local (involving solution properties only on some subset of the overall computational domain) as well as pointwise.

In this talk we concentrate on a simple model problem. Let Ω be a polyhedral domain in $\mathbb{R}^2$ or $\mathbb{R}^3$, and let u solve $-\Delta u = f$ in Ω with $u = 0$ on $\partial\Omega$. Also let $\mathcal{T}_h$ be a shape-regular triangulation of Ω with associated Lagrange finite element space S_k of polynomial degree k. Finally, let $u_h \in S_k$ be the finite element approximation to u.

Residual-type estimates for $\|u - u_h\|_{L_\infty(\Omega)}$ were first proved in [5] and subsequently improved and expanded by various authors. In this talk we present residual-type estimates for global pointwise gradient errors $\|\nabla(u - u_h)\|_{L_\infty(\Omega)}$ and for local pointwise errors $\|\nabla(u-u_h)\|_{L_\infty(D)}$ and $\|u-u_h\|_{L_\infty(D)}$, where D is any subset of Ω. It is well known that bounding local errors requires controlling "pollution effects" of global solution quality upon local solution properties. One thus seeks to define adaptive algorithms that control pollution effects but that require significantly less computational resources than algorithms for controlling corresponding global norms of the error. It should also be noted that if Ω is a non-convex polyhedral domain, then global pointwise control of $\nabla(u - u_h)$ is not possible as ∇u is generally unbounded near reentrant corners.

Singularities arising at vertices of polyhedral domains Ω are a well-known source of pollution in the finite element method. Singularities may in fact pollute not only solution quality (leading to a suboptimal rate of convergence even in areas removed from reentrant corners), but they may also destroy the quality of a posteriori error estimators. To illustrate this point, we note that in order to bound $\|u-u_h\|_{L_2(\Omega)}$ on nonconvex polyhedral domains, one may not simply use the natural residual estimator, but must instead use the more complicated estimator $(\sum_{T\in\mathcal{T}_h} W(T)^2\eta(T)^2)^{1/2}$. Here $W(T)$ is a weight depending on the distance to reentrant corners and the precise nature of the corner singularities, and $\eta(T)$ is the natural L_2-type residual indicator. The construction of $W(T)$ is not difficult (if slightly inconvenient) for simple problems in $\mathbb{R}^2$, but is rather complicated for vertex singularities on polyhedral domains in $\mathbb{R}^3$. Thus one would like to avoid using estimators that require such explicit information about corner singularities.

We explore the use of two templates for controlling pollution and bounding local errors: classical Nitsche-Schatz type local estimates which split the error into a local approximation term and a global pollution term, and sharply local pointwise estimates (proved by Schatz in 1998) which provide smoother control of the pollution error. We first discuss a posteriori counterparts to the latter type of estimate in the case that Ω is convex. Given a subset D of Ω, define $\sigma_D(T) = \frac{h_T}{h_T+dist(D,T)}$. Here $T\in\mathcal{T}_h$ and $h_T = diam(T)$. We then define

$$\mathcal{E}_{D,m} = \max_{T\in\mathcal{T}_h} \sigma_D(T)^m \eta_\infty(T),$$

where $\eta_\infty(T) = h_T\|f+\Delta u_h\|_{L_\infty(T)} + \|[\nabla u_h]\|_{L_\infty(\partial T)}$ is a standard W^1_∞-type residual indicator.

Our results require the following nondegeneracy assumption.

Nondegeneracy assumption $\mathbf{A_D}$: Let $D\subseteq\Omega$. The assumption A_D holds if there exists a point $x_1\in D$ and $\rho>0$ such that $|D^\gamma u(x_1)|\geq C^*>0$ fom some multiindex γ with $|\gamma| = k+1$ and $\|u\|_{W^{k+2}_\infty(B_\rho(x_1))}\leq C^{**}<\infty$. We also define the associated logarithmic factor

$$\ell_{h,u,D,d} = \ln\left[\max\left(\left(\frac{C^{**}+|u|_{C^{1,\alpha}(\overline{D})}}{C^*}\right)^{\frac{k+1}{\alpha}}, \left(\frac{d}{h_{\min}}\right)^{\frac{k+1}{\alpha}}, \left(\frac{1}{\rho}\right)^{\frac{k+1}{\alpha}}\right)\right], \tag{1}$$

where $h_{\min} = \min_{T\in\mathcal{T}_h} h_T$. We then have the following result.

Theorem 1. *Assume that Ω is convex and polyhedral, and let $D\subset\Omega$. Let also the nondegeneracy assumption A_Ω hold. Then*

$$\begin{aligned}\|\nabla(u-u_h)\|_{L_\infty(\Omega)} &\leq C(k,\Omega)\ell_{h,u,\Omega,1}\mathcal{E}_{\Omega,0},\\ \|\nabla(u-u_h)\|_{L_\infty(D)} &\leq \|\sigma_D\nabla(u-u_h)\|_{L_\infty(\Omega)} \leq C(k,\Omega)\ell_{h,u,D,1}\mathcal{E}_{D,1},\end{aligned}$$

and if $k\geq 2$,

$$\|\nabla(u-u_h)\|_{L_\infty(D)} \leq C(k,\Omega)\ell_{h,u,D,1}\mathcal{E}_{D,2}.$$

Here $C(k,\Omega)$ depends on Ω and k. In addition, let ω_T be the patch of elements sharing a face with the element T, and let R_T be any piecewise polynomial of degree k.

We then have the a posteriori lower bound

$$\max_{T\in\mathcal{T}_h} \sigma_D(T)^m(\eta_\infty(T) - h_T\|f + \Delta u_h - R_T\|_{L_\infty(\omega_T)} \le C\|\sigma_D^m \nabla(u-u_h)\|_{L_\infty(\Omega)},$$

where C does not depend on any essential quantities.

Similar results to Theorem 1 above are contained in [1], but they are only valid for $k = 1$ and are not as sharp. One can in addition show that

$$\|u-u_h\|_{L_\infty(D)} \le C(k,\Omega)\ln\frac{1}{h}\max_{T\in\mathcal{T}_h}\sigma_D(T)h_T\eta_\infty(T).$$

Note that this estimate is valid without assuming that a nondegeneracy condition holds.

The analysis of local error estimators is more difficult on nonconvex polyhedral domains. Here we instead use ideas from classical Nitsche-Schatz type local finite element analysis. The following result is contained in [2]. Given a set $D \subset \Omega$ and $d > 0$, we let $D_d = \{x \in \Omega : dist(x, D) < d\}$.

Theorem 2. *Let $\Omega \subset \mathbb{R}^n$, $n = 2, 3$, be polyhedral. Assume that $D \subset \Omega$ and $d > 0$ are such that D_d does not abut any reentrant corners. In addition, assume that the nondegeneracy condition A_D holds. Finally, assume that $u \in C^{1,\alpha}(\overline{D_{\tilde\eta}})$ for some $0 < \alpha < 1$ and $\tilde\eta > 0$. Then for $j \ge 0$ and $1 \le p \le \infty$,*

$$\begin{aligned}\|\nabla(u-u_h)\|_{L_\infty(D)} \le& C_{app}(k)\ell_{h,u,D,d}\max_{T\cap D_d\neq\emptyset}\sigma_D(T)\eta_\infty(T)\\ &+ C_{pol}d^{-1-j-\frac{n}{p}}\|u-u_h\|_{W_p^{-j}(D_d)},\\ \|\nabla(u-u_h)\|_{L_\infty(D)} \le& C_{app}(k)\ell_{h,u,D,d}\max_{T\cap D_d\neq\emptyset}\sigma_D(T)\eta_\infty(T)\\ &+ C_{pol}(\ln\frac{1}{h_{\min}})^2 d^{-1}\max_{T\in\mathcal{T}_h} h_T\eta_\infty(T).\end{aligned}$$

The local bound above is rigorous, but somewhat unwieldy because it involves working with two different norms. Based on Theorem 2, we thus conjecture that even on nonconvex polyhedral domains, $\|\nabla(u-u_h)\|_{L_\infty(D)} \le C(k,\Omega)\ell_{h,u,D,1}\mathcal{E}_{D,1}$. Note that both $\mathcal{E}_{D,1}$ and the final local estimator in Theorem 2 employ η_∞ as their basic building block, with a weight de-emphasizing residual contributions from elements not lying in D. These weights are similar, but not the same. Preliminary computational tests indicate that indeed $\|\nabla(u-u_h)\|_{L_\infty(D)} \le C(k,\Omega)\ell_{h,u,D,1}\mathcal{E}_{E,1}$.

In the context of pointwise estimation of function values, it was shown in [5] and subsequent papers that $\|u-u_h\|_{L_\infty(\Omega)} \le C(\ln\frac{1}{h_{\min}})^2 \max_{T\in\mathcal{T}_h} h_T\eta_\infty(T)$ on both nonconvex and convex polyhedral domains. We have used computations and heuristics to explore whether a more local estimator can be established that does not require explicit singularity information. First, computational tests indicate that the estimate

$$\|u-u_h\|_{L_\infty(D)} \le C\max_{T\in\mathcal{T}_h}\sigma_D(T)h_T\eta_\infty(T)$$

does *not* hold on nonconvex polyhedral domains (recall that we have proved that this estimate *does* hold on convex polyhedral domains). Thus the estimator is "polluted" by strong corner singularities. However, final computational tests indicate

that $\|u - u_h\|_{L_\infty(D)} \leq C \max_{T\in\mathcal{T}_h} \sigma_D(T)^{1/2} h_T \eta_\infty(T)$. Heuristics involving the maximum strength of corner singularities also indicate that this estimate should hold.

References

[1] A. Demlow, *Localized pointwise a posteriori error estimates for gradients of piecewise linear finite element approximations to second-order quasilinear elliptic problems*, SIAM J. Numer. Anal. **44** (2006), 494–514.

[2] A. Demlow, *Local a posteriori estimates for pointwise gradient errors in finite element methods for elliptic problems*, Math. Comp. **76** (2007), 19–42.

[3] X. Liao and R.H. Nochetto, *Local a posteriori error estimates and adaptive control of pollution effects*, Numer. Methods Partial Differential Equations **19** (2003), pp. 421–442.

[4] R. Lipton, *Bounds on the distribution of extreme values for the stress in composite materials*, J. Mech. Phys. Solids **52** (2004), 1053–1069.

[5] R. H. Nochetto, *Pointwise a posteriori error estimates for elliptic problems on highly graded meshes*, Math. Comp. **64** (1995), 1–22.

[6] E. Svensson, *Computational characterization of mixing in flows*, PhD thesis, Chalmers University of Technology and Göteborg University, 2006.

Adaptive finite element methods for fluid-structure interaction problems based on an Eulerian variational formulation

Thomas Dunne

Computational fluid dynamics and computational structure mechanics are two major areas of numerical simulation of physical systems. With the introduction of high performance computing it has become possible to tackle systems with a coupling of fluid and structure dynamics. General examples of such fluid-structure interaction (FSI) problems are flow transporting elastic particles (particulate flow), flow around elastic structures (airplanes, submarines) and flow in elastic structures (haemodynamics, transport of fluids in closed containers). In all these settings the dilemma in modeling the coupled dynamics is that the fluid model is normally based on an Eulerian perspective in contrast to the usual Lagrangian approach for the solid model. This makes the setup of a common variational description difficult. However, such a variational formulation of FSI is needed as the basis of a consistent approach to residual-based a posteriori error estimation and mesh adaptation as well as to the solution of optimal control problems by the Euler-Lagrange method.

Combining the Eulerian and the Lagrangian setting for describing FSI involves conceptional difficulties. On the one hand the fluid domain itself is time-dependent and depends on the deformation of the structure domain. On the other hand, for the structure the fluid boundary values (velocity and the normal stress) are needed. In both cases values from the one problem are used for the other, which is costly and can lead to a drastic loss of accuracy. A common approach to dealing with this problem is to separate the two models, solve each one after the other, and so converge iteratively to a solution, which satisfies both together with the interface

conditions Solving the separated problems serially multiple times is referred to as a 'partitioned approach'. For advanced examples of this approach see [BuSc+06].

A basic partitioned approach does not contain a variational equation for the fluid-structure interface. To achieve this, usually an auxiliary unknown coordinate transformation function ζ_f is introduced for the fluid domain. With its help the fluid problem is rewritten as one on the transformed domain, which is fixed in time. Then, all computations are done on the fixed reference domain and as part of the computation the auxiliary transformation function ζ_f has to be determined at each time step.

Such, so-called 'arbitrary Lagrangian-Eulerian' (ALE) methods are also treated in the authors doctoral dissertation [Du07a]. Multiple good examples and quantitative results can be found in [BuSc+06], e.g. [HronTurek206, TuHr06].

Both, the partitioned and the transformation approach overcome the Euler-Lagrange discrepancy by explicitly tracking the fluid-structure interface. This is done by mesh adjustment or aligning the mesh to match the interface and is generally referred to as 'interface tracking'. Both methods leave the structure problem in its natural Lagrangian setting.

We follow the alternative (and to our knowledge new) way of posing the fluid as well as the structure problem in a fully Eulerian framework. In the Eulerian setting a phase variable is employed on the fixed mesh to distinguish between the different phases, liquid and solid. This approach to identifying the fluid-structure interface is generally referred to as 'interface capturing', a method commonly used in the simulation of multiphase flows, [JoRe93a, JoRe93b]. Examples for the use of such a phase variable are the Volume of Fluid (VoF) method [HiNi81] and the Level Set (LS) method [OsherSethian, Sethian99]. In the classical LS approach the distance function has to continually be reinitialized, due to the smearing effect by the convection velocity in the fluid domain. This makes the use of the LS method delicate for modeling FSI problems particularly in the presence of cornered structures. To cope with this difficulty, we introduce a variant of the LS method that makes reinitialization unnecessary and which can easily cope with cornered structures.

The method we describe does not depend on the specific structure model. The key variable in structure dynamics is the deformation, and since this depends on the deflection, it is understandable why structure dynamics is preferably described in the Lagrangian frame. To be able to describe the deformations in the Eulerian frame, we introduce the 'Initial Positions set' (IP set) of all structure points. This set is then transported with the structure velocity in each time step. Based on the IP set points and their Eulerian coordinates the displacement is now available in an Eulerian sense. Also its gradient has to be rewritten appropriately. Since the fluid-structure interface will be crossing through cells, we will have to also transport the IP set in the fluid domain.

If we were to use the fluid velocity for the convection of the IP set, this would lead to entanglement of the respective displacements, which would 'wreak havoc' on the interface cells. This is a known problem with LS approaches. A common

way for fixing this problem has been to occasionally fix the LS field between the time steps. The problem with this approach is that the variational formulation is no longer consistent. As an alternative, we harmonically continue the structure velocity into the fluid domain. In the fluid domain we then use this velocity for the convection of the IP set. Since an IP set is available in both domains, we can always at each point determine if it belongs to the fluid or solid part of the model.

Again, this approach is similar to the LS approach. But when developing a complete variational formulation the two key characteristics of the LS approach also become the main cause of concern: reinitialization and the signed distance function. Although the problem of reinitialization here can also be avoided by using an harmonically extended velocity, the trouble concerning corner approximation persists. In contrast to this, by using an initial position set, we are deforming a virtual mesh of the structure, which is extended into the whole domain.

Based on the Eulerian variational formulation of the FSI system, we use the 'dual weighted residual' (DWR) method, described in [BeRa95, BeRa01], to derive 'goal-oriented' a posteriori error estimates. The evaluation of these error estimates requires the approximate solution of a linear dual variational problem. The resulting a posteriori error indicators are then used for automatic local mesh adaption. The full application of the DWR method to FSI problems requires a Galerkin discretization in space as well as in time. Due to the use of a difference scheme in time, we are limited to 'goal-oriented' mesh adaptation in computing steady states or (somewhat heuristically) to quasi-steady states within the time stepping process.

The method for computing FSI described is validated at a stationary model problem that is a lid-driven cavity involving the interaction of an incompressible Stokes fluid with an incompressible neo-Hookean solid. Then, as a more challenging test the self-induced oscillation of a thin elastic bar immersed in an incompressible fluid is treated (FLUSTRUK-A benchmark described in [TuHr06] and [HronTurek206]). For this test problem, our fully Eulerian method is also compared against a standard 'arbitrary Lagrangian-Eulerian' (ALE) approach. The possible potential of the fully Eulerian formulation of the FSI problem is indicated by its good behavior for large structure deformations.

Further details and results concerning Eulerian and ALE-Formulations of FSI problems as well as adaptivity for FSI problems can be found in the authors doctoral dissertation [Du07a] as well as in [DuRa06, BuSc+06]. All computations and visualizations were done using the flow-solver package GASCOIGNE [Ga] and the graphics package VISUSIMPLE [BeDu06, Vi].

References

[BeDu06] R. Becker, Th. Dunne, *VisuSimple: An interactive open source visualization utility for scientific computing*, in "Reactive Flows, Diffusion and Transport: From Experiments via Mathematical Modeling to Numerical Simulation and Optimization, Final Report of SFB (Collaborative Research Center) 359" Jäger, Willi; Rannacher, Rolf; Warnatz, Jürgen (Eds.) Springer; (October 31, 2006) 676 p., ISBN-10: 3-540-28379-X ISBN-13: 978-3-540-28379-9 . See [Vi].

[BeRa95] R. Becker and R. Rannacher, Weighted a-posteriori error estimates in FE methods, Lecture ENUMATH-95, Paris, Sept. 18-22, 1995, in: *Proc. ENUMATH-97*, (H.G. Bock, et al., eds), pp. 621-637, World Scientific Publ., Singapore, 1998.

[BeRa01] R. Becker and R. Rannacher, An optimal control approach to error estimation and mesh adaption in finite element methods, *Acta Numerica 2000* (A. Iserles, ed.), pp. 1-101, Cambridge University Press, 2001.

[BuSc+06] H.-J. Bungartz, M. Schäfer (Eds.), *Fluid-Structure Interaction Modelling, Simulation, Optimization*, Springer Series: Lecture Notes in Computational Science and Engineering, Vol. 53 2006, VIII, 394 p., 251 illus., Softcover ISBN-10: 3-540-34595-7, ISBN-13: 978-3-540-34595-4

[Du06a] Th. Dunne *An Eulerian approach to fluid-structure interaction and goal-oriented mesh refinement*, Proc. "Finite Elements for Flow Problems (FEF05)", IACM Special Interest Conference supported by ECCOMAS, April 4-6, 2005, Swansea, Wales, UK, appeared in Int. J. Numer. Meth. Fluids 2006; 51: 1017-1039.

[Du06b] Th. Dunne *Adaptive Finite Element Approximation of Fluid-Structure Interaction Based on an Eulerian Variational Formulation*, Proc. "European Conference on Computational Fluid Dynamics (ECCOMAS CFD 2006)", September 5-8, 2006, Egmond aan Zee, The Netherlands.

[Du07a] Th. Dunne. *Adaptive Finite Element Approximation of Fluid-Structure Interaction Based on Eulerian and Arbitrary Lagrangian-Eulerian Variational Formulations* Institute of Applied Mathematics, University of Heidelberg, doctoral dissertation, 2007.

[DuRa06] Th. Dunne., R. Rannacher, *Adaptive finite element simulation of fluid structure interaction based on an Eulerian variational formulation*, p. 371-386, in H.-J. Bungartz, M. Schäfer (Eds.) *Fluid-Structure Interaction Modelling, Simulation, Optimization*, Springer Verlag, (2006). [BuSc+06]

[Ga] GASCOIGNE, A C++ numerics library for scientific computing, `http://gascoigne.uni-hd.de/`.

[HiNi81] C. W. Hirt and B. D. Nichols, Volume of Fluid (VOF) method for the dynamics of free boundaries. *Journal of Computational Physics* 39, 201-225 (1981).

[HronTurek206] J. Hron, S. Turek, *A Monolithic FEM/Multigrid Solver for an ALE Formulation of Fluid-Structure Interaction with Applications in Biomechanics*, p. 146-170, in H.-J. Bungartz, M. Schäfer (Eds.) *Fluid-Structure Interaction Modelling, Simulation, Optimization*, Springer Verlag, (2006). [BuSc+06]

[JoRe93a] D. D. Joseph and Y. Y. Renardy, *Fundamentals of two-fluid dynamics. Part I*, Springer, New York, 1993. Math. Theory and Applications.

[JoRe93b] D. D. Joseph and Y. Y. Renardy, *Fundamentals of two-fluid dynamics. Part II*, Springer, New York, 1993.

[OsherSethian] S. Osher and J. A. Sethian, Propagation of fronts with curvature based speed: algorithms based on Hamilton-Jacobi formulations, *Journal of Computational Physics* 79, 12 (1988).

[Sethian99] J.A. Sethian, *Level set methods and fast marching methods.* Cambridge University Press, 1999.

[TuHr06] S. Turek, J. Hron, *Proposal for Numerical Benchmarking of Fluid-Structure Interaction between an Elastic Object and Laminar Incompressible Flow* p. 371-386, in H.-J. Bungartz, M. Schäfer (Eds.) *Fluid-Structure Interaction Modelling, Simulation, Optimization*, Springer Verlag, (2006). [BuSc+06]

[Vi] VISUSIMPLE, An open source interactive visualization utility for scientific computing, `http://visusimple.uni-hd.de/` . See [BeDu06].

Functional majorants for distributed optimal control problems with control constraints

Alexandra Gaevskaya
(joint work with Ronald H.W. Hoppe and Sergey Repin)

We present a new approach to the a posteriori analysis of distributed optimal control problems associated with elliptic type partial differential equations with control constraints. In resent years, this question has been actively developed in the framework of the residual based and goal-oriented approaches for a posteriori control of the associated PDE (see, e.g., [1, 3, 5]). Our results are based on functional type a posteriori estimates that provide sharp bounds for the error with respect to any feasible approximation of the state (see, e.g., [6, 7]). Some of the results for the a posteriori analysis of optimal control problems based on functional type error estimates are presented in [2] and [4].

Let $\Omega \in \mathbb{R}^n$ be a bounded Lipschitz domain. We consider the optimal control problem of the following form:

Problem P. Given $y^d \in H_0^1(\Omega), u^d \in L_2(\Omega)$, $f \in L_2(\Omega)$, $\psi \in L_\infty(\Omega)$, and $a > 0$, consider the distributed control problem

$$\begin{aligned} &\text{minimize} \quad J(y,u) := \frac{1}{2}\,\|\nabla(y-y^d)\|^2 + \frac{a}{2}\,\|u-u^d\|^2 \\ &\text{over} \qquad (y,u) \in H_0^1(\Omega)\times L^2(\Omega), \\ &\text{subject to} \; -\Delta\, y = u+f \quad \text{a.e. in } \Omega, \\ &\qquad\qquad u \in K = \{v \in V \mid v \le \psi \text{ a.e. in } \Omega\}\,. \end{aligned}$$

Let y_{u+f} be the state of the system corresponding to the conrol u, i.e.,

$$\begin{aligned} -\Delta y_{u+f} &= u+f \qquad \text{in} \quad \Omega, \\ y_{u+f} &= 0 \qquad \text{on} \quad \partial\Omega. \end{aligned}$$

By (y^*,u^*) (with $y^* := y_{u^*+f}$) we denote the exact solution of Problem P.

Using the functional type a posteriori estimates, we derive guaranteed and computable two-sided estimates for the optimal value of the cost functional. In particular, for any conforming approximation of the state and the control $(y,u) \in H_0^1(\Omega)\times K$ there holds

$$J^{\ominus}(y;w) \le J(y^*,u^*) \le J(y_{u+f},u) \le J^{\oplus}(y,u;\beta;\tau), \tag{2}$$

where the auxiliary functions $w \in H_0^1(\Omega)$, $\tau \in H_{\mathrm{div}}(\Omega,\mathbb{R}^n)$ and parameter $\beta > 0$ can be taken arbitrary.

The two-sided estimates for the cost functional (2) give rise to guaranteed and computable upper estimate for the error in the solution of the optimal control problem measured in the combined norm

$$|[u-u^*]|^2 := \frac{1}{2}\|\nabla y_{u+f} - \nabla y_{u^*+f}\|^2 + \frac{a}{2}\|u-u^*\|^2.$$

Namely, for any control $u \in K$ and state $y \in H_0^1(\Omega)$ there holds

$$|[u-u^*]|^2 \le J^{\oplus}(y,u;\beta;\tau) - J^{\ominus}(y;w), \tag{3}$$

with arbitrary $\tau \in H_{\mathrm{div}}(\Omega, \mathbb{R}^n), w \in H_0^1(\Omega)$ and $\beta > 0$.

The functionals $J^{\oplus}(y, u; \beta; \tau)$ and $J^{\ominus}(y; w)$ ('the majorant' and 'the minorant' for the cost functional, respectively) are quadratic with respect to the auxiliary arguments τ and w. They involve only known functions and parameters and can be evaluated in the discrete setting. Therefore, the estimate (2) can be used to find guaranteed and computable two-sided bounds for the cost functional when the optimization problem is solved by known methods.

The estimate (3) allows to compute a guaranteed bound for the error in the solution of the optimal control problem measured in combined norm and provides information about distribution of the error over the computational domain.

References

[1] R. Becker, R. Rannacher. An optimal control approach to error estimation and mesh adaptation in finite element methods. In: Acta Numerica (A. Iserles, ed.), 10: 1–102, Cambridge University Press, 2001.

[2] A. Gaevskaya, R.H.W. Hoppe, and S. Repin. A Posteriori Estimates for Cost Functionals of Optimal Control Problems. to appear in Proc. ENUMATH 2005 Conf., Santiago de Compostela, July 18-22, 2005.

[3] A. Gaevskaya, R.H.W.Hoppe, Y. Iliash, and M. Kieweg. A posteriori error analysis of adaptive finite element methods for control constrained distributed and boundary control problems. Proc. Conf. Advances in Scientific Computing, Moscow, Russia (O. Pironneau et al.; eds), Russian Academy of Sciences, Moscow, 2006

[4] A. Gaevskaya, R.H.W. Hoppe, and S. Repin. Functional Approach to a Posteriori Error Estimation for Elliptic Optimal Control Problems with Distributed Control. Journal of Mathematical Sciences, Vol. 144, No. 6, 2007, pp. 4535–4548

[5] R. Li, W. Liu, H. Ma, and T. Tang. Adaptive finite element approximation for distributed optimal control problems. SIAM J. Control Optim. Vol. 41, No. 5 (2002), 1321–1349

[6] S. Repin. *A posteriori error estimation for nonlinear variational problems by duality theory.* Zapiski Nauchn. Semin. POMI,**243** (1997), 201–214.

[7] S. Repin, Two-Sided Estimates of Deviation from Exact Solutions of Uniformly Elliptic Equations, Amer. Math. Soc. Transl., (2) Vol. 209 (2003), 143–171.

A posteriori error estimates for viscous flow problems with rotation

Elena Gorshkova

(joint work with Pekka Neittaanmäki and Sergey Repin)

In this work we consider linear incompressible viscous flow problem with rotation. Such problem are physically motivated, e.g., by geophysics, when movement of the oceanic mass has to be calculated. Certainly, this model is rather contracted and does not take into account nonlinear effects. However, we believe that the present work is a necessary step in the creation of reliable methods for more complicated system in the theory of rotation fluids (see [1], [2]).

Consider the following system

$$-\nu \triangle u + \Omega \times u = f - \nabla p \quad \text{in } \mathcal{D}, \tag{1}$$

$$\operatorname{div} u = 0 \quad \text{in } \mathcal{D}, \tag{2}$$

$$u = u_0 \quad \text{on } \partial\mathcal{D}. \tag{3}$$

Here $\nu > 0$ is the viscosity parameter, $f \in L_2(\mathcal{D}, \mathbb{R}^n)$ is a given vector-valued function, p is the pressure function and $u_0 \in H^1(\mathcal{D}, \mathbb{R}^n)$ defines the Dirichlet boundary conditions on $\partial\mathcal{D}$. It is assumed that $\operatorname{div} u_0 = 0$.

The new a posteriori error estimate for the system (1-3) was recently obtained in [5]. The error error estimate was obtained with the help of the functional method of analysis of the boundary value problem. Such approach was first presented in [6].

Assume that

$$v \in \overset{o}{H}{}^1(\mathcal{D}, \mathbb{R}^n) + u_0 := \left\{ w \in H^1(\mathcal{D}, \mathbb{R}^n) \;||\; w = \tilde{w} + u_0, \tilde{w} \in \overset{o}{H}{}^1(\mathcal{D}, \mathbb{R}^n) \right\}$$

is some approximate solution obtained by any numerical method. Then the difference between exact and approximate solution can be estimated in the following way:

$$\nu\|\nabla(u-v)\| \le \|\tau - \nu\nabla v\| + c_{\mathcal{D}}\|f + \operatorname{div}\tau - \Omega \times v - \nabla q\| + \\ + (2\nu + |\Omega| c_{\mathcal{D}}) \frac{1}{\mathcal{C}_{LBB}} \|\operatorname{div} v\|. \tag{4}$$

Here $c_{\mathcal{D}}$ is the constant from the Friedrichs inequality and $\mathcal{C}_{LBB}$ is the constant from Ladyzhenskaya-Babuška-Brezzi (inf-sup) inequality.

Let us note, then if rotation parameter is equal to zero, then the problem (1-3) coincides with the Stokes problem, and the error estimate (4) coincide with the a posteriori error estimate for the Stokes problem obtained in [7]. In our previous research we have numerically tested the estimate (see [3]) and compared with other types of a posteriori error estimate (see [4]).

The functional in the right hand side of (4) majorize the deviation of the approximate solution from the exact one, therefore it is called *the error majorant*.

For practical purposes, it is more convenient to use the above error majorant in a somewhat different form. Let us square both parts of the (4) and use the Young's inequalities with positive scalar parameters α_1, α_2, α_3. Thus, we obtain

$$\nu^2\|\nabla(u-v)\|^2 \le (1 + \alpha_1 + \alpha_2)\|\nu\nabla v - \tau\|^2 + \\ + (1 + \frac{1}{\alpha_1} + \alpha_3) C_\Omega^2 \|\operatorname{div}\tau + f - \nabla q - \Omega \times v\|^2 + \\ + (1 + \frac{1}{\alpha_2} + \frac{1}{\alpha_3})(2\nu + |\Omega| c_{\mathcal{D}})^2 \frac{1}{\mathcal{C}_{LBB}^2} \|\operatorname{div} v\|^2. \tag{5}$$

Optimal value for scalar parameters α_i can be stated analytically.

We note that the right-hand sides of (5) contain only known data (v, ν, f, Ω, $\mathcal{D}$) and the functions (α_i, τ, q), which are in our disposal. Therefore, they are directly computable. It is clear, that (α_i, τ, q) should be selected in order to minimize the right-hand side of the error majorant.

Minimization of the right-hand side of (5) is a problem of minimization of quadratic functional, that is reduced to a system of linear simultaneous equations. We would like to underline, that it is not necessary to find the exact minimizer of this system. Starting from the initial approach we can use some iterative numerical

procedure. On the each iteration step, the value of the error majorant give an upper bound of the error. A function obtained at the end of minimization process yield an error indicator.

Finally in this work, we present a series of numerical tests and demonstrate efficiency of the error estimate proposed in estimation overall accuracy of the approximate solution as well as the the error indication, necessary for the further mesh adaptation.

List of references.

[1] A. Babin, A. Mahalov, and B. Nicolaenko; "Global splitting, integrability and regularity of 3D Euler and Navier-Stokes equations for uniformly rotating fluids", European Journal of Mechanics, 15, (1996), pp. 291–300.

[2] A. Babin, A. Mahalov, and B. Nicolaenko; "Global regularity of 3D rotating Navier-Stokes equations for resonant domains", Indiana University Mathematics Journal, 48, (1999), pp. 1133–1176.

[3] E. Gorshkova and S. Repin; "Error control of the approximate solution to the Stokes equation using a posteriori error estimates of functional type". In *European Congress on Computational Methods in Applied Sciences and Engineering, ECCOMAS 2004, P.Neittaanmäki, T. Rossi, K. Majava and O. Pironeau (eds.), O. Nevanlinna and R. Rannacher (assoc. eds.), Jyväskylä, 24-28 July, 2004* (electronic).

[4] E. Gorshkova, P. Neittaanmaki, S. Repin; "Comparative study of the a posteriori error estimators for the Stokes Problem", Numerical Mathematics and Advanced Application (ENUMATH 2005), Springer-Veglar, Berlin, Heidelberg, 2006, pp. 252–259.

[5] E. Gorshkova, A. Mahalov, P. Neittaanmaki, S. Repin; "A posteriori error estimates for viscous fluids with rotation", J.Math.Sci.,142 (2007), no. 1, pp. 1749–1762.

[6] S. Repin; "A posteriori error estimation for nonlinear variational problems by duality theory"; Zapiski Nauchnych Seminarov V.A. Steklov Math. Inst. in St.-Peterburg, 243(1997) 201–214(in Russian);English transl.: J.Math.Sci. (New York) 99 (2000), no. 1, pp. 927–935.

[7] S. Repin; "A posteriori estimates for the Stokes problem". J.Math.Sci., 109 (2002), no. 5, pp. 1950–1964.

Model adaptivity for plates

Peter Hansbo
(joint work with Mats G. Larson)

The Reissner plate model is described by the following partial differential equations:

$$
\begin{aligned}
-\nabla\cdot\boldsymbol{\sigma}(\boldsymbol{\theta}) - \kappa\, t^{-2}\,(\nabla u - \boldsymbol{\theta}) = 0 \quad &\text{in} \quad \Omega\subset\mathbb{R}^2,\\
-\nabla\cdot\big(\kappa\, t^{-2}\,(\nabla u - \boldsymbol{\theta})\big) = g \quad &\text{in} \quad \Omega,
\end{aligned}
\tag{1}
$$

where u is the transverse displacement, $\boldsymbol{\theta}$ is the rotation of the median surface, t is the thickness, $t^3\, g$ is the transverse surface load, and

$$\boldsymbol{\sigma}(\boldsymbol{\theta}) := 2\mu\boldsymbol{\varepsilon}(\boldsymbol{\theta}) + \lambda\nabla\cdot\boldsymbol{\theta}\,\mathbf{1}$$

is the moment tensor. Here, $\mathbf{1}$ is the identity tensor and $\boldsymbol{\varepsilon}$ is the curvature tensor with components

$$\varepsilon_{ij}(\boldsymbol{\theta}) = \frac{1}{2}\left(\frac{\partial\theta_i}{\partial x_j} + \frac{\partial\theta_j}{\partial x_i}\right).$$

The constitutive parameters are given by the relations $\kappa = E\,k/(2(1+\nu))$, $\mu := E/(6(1+\nu))$, and $\lambda := \nu E/(12(1-\nu^2))$, where E and ν are the Young's modulus and Poisson's ratio, respectively, and $k\approx 5/6$ is a shear correction factor.

The differential equations describing the Reissner plate model can be derived from minimization of the sum of the bending energy, the shear energy, and the potential of the surface load,

$$\mathcal{R}(u,\boldsymbol{\theta}) = \frac{1}{2}a(\boldsymbol{\theta},\boldsymbol{\theta}) + b(\nabla u - \boldsymbol{\theta}, \nabla u - \boldsymbol{\theta}) - \int_\Omega g\, u\, d\Omega \tag{2}$$

where

$$a(\boldsymbol{\theta},\boldsymbol{\vartheta}) = \int_\Omega \boldsymbol{\sigma}(\boldsymbol{\theta}) : \boldsymbol{\varepsilon}(\boldsymbol{\vartheta})\, d\Omega \quad\text{and}\quad b(\boldsymbol{\theta},\boldsymbol{\vartheta}) = \int_\Omega t^{-2}\boldsymbol{\theta}\cdot\boldsymbol{\vartheta}\, d\Omega.$$

In the limit $t\to 0$ we obtain the Kirchhoff model which corresponds to minimization of

$$\mathcal{K}(u) = \frac{1}{2}a(\nabla u,\nabla u) - \int_\Omega g\, u\, d\Omega. \tag{3}$$

Note that in this case $\boldsymbol{\theta} = \nabla u$.

Our goal is to deduce *a posteriori* error estimates for both the discretization error and the model error between the Kirchhoff and the Reissner model. We then need a finite element method that can be used in both cases. To define such a method we introduce a tirangulation $\mathcal{T}$ of Ω into affine simplices T, as well as the set of edges in the mesh, $\mathcal{E} = \{E\}$, and we split $\mathcal{E}$ into two disjoint subsets

$$\mathcal{E} = \mathcal{E}_I \cup \mathcal{E}_B,$$

where $\mathcal{E}_I$ is the set of edges in the interior of Ω and $\mathcal{E}_B$ is the set of edges on the boundary. Further, with each edge we associate a fixed unit normal $\boldsymbol{n}$ such that for edges on the boundary $\boldsymbol{n}$ is the exterior unit normal. We denote the jump of a function $\boldsymbol{v}$ at an edge E by $[\boldsymbol{v}] = \boldsymbol{v}^+ - \boldsymbol{v}^-$ for $E\in\mathcal{E}_I$ and $[\boldsymbol{v}] = \boldsymbol{v}^+$ for $E\in\mathcal{E}_B$,

and the average $\langle \boldsymbol{v} \rangle = (\boldsymbol{v}^+ + \boldsymbol{v}^-)/2$ for $E \in \mathcal{E}_I$ and $\langle \boldsymbol{v} \rangle = \boldsymbol{v}^+$ for $E \in \mathcal{E}_B$, where $\boldsymbol{v}^\pm = \lim_{\epsilon \downarrow 0} \boldsymbol{v}(\boldsymbol{x} \mp \epsilon \boldsymbol{n})$ with $\boldsymbol{x} \in E$.

Our method can now be formulated as follows: find $(u_h, \boldsymbol{\theta}_h) \in V_h \times \boldsymbol{W}_h$, where

$$V_h = \{v \in H_0^1(\Omega) \cap C^0(\Omega) : \ v|_T \in P^2(T) \text{ for all } T \in \mathcal{T}\},$$

and

$$\boldsymbol{W}_h := \{\boldsymbol{\vartheta} \in [L^2(\Omega)]^2 : \ \boldsymbol{\vartheta}|_T \in [P^1(T)]^2 \text{ for all } T \in \mathcal{T}\},$$

such that

$$a_h(\boldsymbol{\theta}_h, \boldsymbol{\vartheta}) + b(\nabla u_h - \boldsymbol{\theta}_h, \nabla v - \boldsymbol{\vartheta}) = (g, v) \tag{4}$$

for all $(v, \boldsymbol{\vartheta}) \in V_h \times \boldsymbol{W}_h$. In (4) the bilinear form $a_h(\cdot, \cdot)$ is defined on $\boldsymbol{W}_h \times \boldsymbol{W}_h$ as follows

$$\begin{aligned} a_h(\boldsymbol{\theta}, \boldsymbol{\vartheta}) = &\sum_{T \in \mathcal{T}} (\boldsymbol{\sigma}(\boldsymbol{\theta}), \boldsymbol{\varepsilon}(\boldsymbol{\vartheta}))_T - \sum_{E \in \mathcal{E}_I \cup \mathcal{E}_B} (\langle \boldsymbol{n} \cdot \boldsymbol{\sigma}(\boldsymbol{\theta}) \rangle, [\boldsymbol{\vartheta}])_E + (\langle \boldsymbol{n} \cdot \boldsymbol{\sigma}(\boldsymbol{\vartheta}) \rangle, [\boldsymbol{\theta}])_E \\ &+ (2\mu + 3\lambda)\, \gamma \sum_{E \in \mathcal{E}_I \cup \mathcal{E}_B} h_E^{-1} ([\boldsymbol{\theta}], [\boldsymbol{\vartheta}])_E \end{aligned}$$

for all $\boldsymbol{\theta}, \boldsymbol{\vartheta} \in \boldsymbol{W}_h$. Here γ is a positive constant and h_E is defined by

$$h_E = \left(|T^+| + |T^-|\right) / (2\,|E|) \quad \text{for } E = \partial T^+ \cap \partial T^-, \tag{5}$$

with $|T|$ the area of T, on each edge.

Setting $\boldsymbol{\theta}_h = \nabla u_h$ and $\boldsymbol{\vartheta} = \nabla v$ we get the following method: find $u_h \in V_h$ such that

$$a_h(\nabla u_h, \nabla v) = (g, v) \tag{6}$$

for all $v \in V_h$. It is possible to show that the suggested finite element method is stable and convergent in both cases (cf. [1, 2]).

Using *a posteriori* analysis, together with *a priori* stability of the continuous problem, we can deduce an estimate of the type

$$\begin{aligned} \frac{(u - u_h, \psi)}{\|\psi\|_{H^{-1}(\Omega)} + t\|\psi\|_{L_2(\Omega)}} \le C\big(&(h^3 + th^2)\|R_1(\theta^h)\|_{L_2(\Omega)} \\ &+ th\|R_2(\theta^h - \nabla u^h)\|_{L_2(\Omega)} + t\|R_2(\theta^h - \nabla u^h)\|_{H^{-1}(\Omega)}\big) \end{aligned}$$

(for ψ arbitrary) where R_1 describes the imbalance between moments and external load and R_2 the imbalance between moments and shear forces. Details will be given in a forthcoming paper.

References

[1] G. Engel, K. Garikipati, T. J. R. Hughes, M. G. Larson, L. Mazzei, R. L. Taylor *Continuous/discontinuous finite element approximations of fourth-order elliptic problems in structural and continuum mechanics with applications to thin beams and plates, and strain gradient elasticity*, Comput. Methods Appl. Mech. Engrg. **191** (2002), 3669–3750.

[2] P. Hansbo, M. G. Larson, *A P^2-continuous, P^1-discontinuous finite element method for the Mindlin-Reissner plate problem*, in: Numerical Mathematics and Advanced Applications: ENUMATH 2001, F. Brezzi, A. Buffa, S. Corsaro, and A. Murli (Eds.), Springer, 2003, pp. 765-774.

DG discretizations for compressible flows: Adjoint consistency analysis, error estimation and adaptivity

Ralf Hartmann

1. Adjoint consistency - in addition to consistency - is the key requirement for discontinuous Galerkin (DG) discretizations to be of optimal order in L^2 as well as measured in terms of target functionals $J(\cdot)$. If the primal and adjoint solutions are sufficiently smooth, the order of convergence in J for an adjoint consistent discretization is twice the order of an adjoint inconsistent discretization (order doubling). In this talk we provide a general framework, see [3, 4], for analyzing the adjoint consistency of DG discretizations. We collect several conclusions which can be drawn from analyzing the adjoint consistency property of DG discretizations of the linear advection equation, Poisson's equation and the compressible Euler and Navier-Stokes equations. Consider the linear problem and linear target functional

$$Lu = f \quad \text{in } \Omega, \qquad\qquad Bu = g \quad \text{on } \Gamma, \tag{1}$$

$$J(u) = \int_\Omega j_\Omega \, u \, \mathrm{d}\mathbf{x} + \int_\Gamma j_\Gamma \, Cu \, \mathrm{d}s, \tag{2}$$

where L denotes a linear differential operator on Ω, and B and C denote linear differential (boundary) operators on Γ. The target functional $J(\cdot)$ in (2) is said to be *compatible* with (1), provided following compatibility condition holds

$$(Lu, z)_\Omega + (Bu, C^* z)_\Gamma = (u, L^* z)_\Omega + (Cu, B^* z)_\Gamma, \tag{3}$$

where L^*, B^* and C^* denote the adjoint operators to L, B and C. Then the (continuous) adjoint problem associated to (1), (2) is given by

$$L^* z = j_\Omega \quad \text{in } \Omega, \qquad\qquad B^* z = j_\Gamma \quad \text{on } \Gamma. \tag{4}$$

Let (1) be discretized as follows: find $u_h \in V_h$ such that

$$\mathcal{B}(u_h, v_h) = \mathcal{F}(v_h) \quad \forall v_h \in V_h, \tag{5}$$

Then, the discretization (5) is *consistent* if the exact solution $u \in V$ to the primal problem (1) satisfies: $\mathcal{B}(u, v) = \mathcal{F}(v)$ for all $v \in V$. Similarly, the discretization (5) is *adjoint consistent* if the exact solution $z \in V$ to the continuous adjoint problem (4) satisfies: $\mathcal{B}(w, z) = J(w)$ for all $w \in V$.

Analoguously, for a nonlinear problem and nonlinear target functional

$$Nu = 0 \quad \text{in } \Omega, \qquad\qquad Bu = 0 \quad \text{on } \Gamma, \tag{6}$$

$$J(u) = \int_\Omega j_\Omega(u) \, \mathrm{d}\mathbf{x} + \int_\Gamma j_\Gamma(Cu) \, \mathrm{d}s, \tag{7}$$

where N is a nonlinear differential operator and B is a (possibly nonlinear) boundary operator, the continuous adjoint problem is given by

$$(N'[u])^* z = j'_\Omega[u] \quad \text{in } \Omega, \qquad\qquad (B'[u])^* z = j'_\Gamma[Cu] \quad \text{on } \Gamma. \tag{8}$$

Let $\mathcal{N} : V \times V \to \mathbb{R}$ be a semi-linear form, such that the nonlinear problem (6) is discretized as follows: find $u_h \in V_h$ such that

$$\mathcal{N}(u_h, v_h) = 0 \quad \forall v_h \in V_h. \tag{9}$$

The corresponding discrete adjoint problem is given by: find $z_h \in V_h$ such that

$$\mathcal{N}'[u_h](w_h, z_h) = J'[u_h](w_h) \quad \forall w_h \in V_h, \tag{10}$$

where $\mathcal{N}'[u]$ denotes the Fréchet derivatives of $\mathcal{N}(u, v)$ with respect to u. The discretization (9) is *consistent* if the exact solution $u \in V$ to the primal problem (6) satisfies following equation:

$$\mathcal{N}(u, v) = 0 \quad \forall v \in V. \tag{11}$$

Furthermore, the discretization (9) is *adjoint consistent* if the exact solution $z \in V$ to the adjoint problem (8) satisfies following equation:

$$\mathcal{N}'[u](w, z) = J'[u](w) \quad \forall w \in V, \tag{12}$$

In other words, a discretization is adjoint consistent if the discrete adjoint problem is a consistent discretization of the continuous adjoint problem.

For analysing adjoint consistency we rewrite the discrete adjoint problem (10) in element-based adjoint residual form: find $z_h \in V_h$ such that

$$\sum_{\kappa \in \mathcal{T}_h} \int_\kappa w_h \, R^*[u_h](z_h) \, \mathrm{d}\mathbf{x} + \sum_{\kappa \in \mathcal{T}_h} \int_{\partial\kappa \setminus \Gamma} w_h \, r^*[u_h](z_h) \, \mathrm{d}s + \int_\Gamma w_h \, r^*_\Gamma[u_h](z_h) \, \mathrm{d}s = 0, \tag{13}$$

for all $w_h \in V_h$, where $R^*[u_h](z_h)$, $r^*[u_h](z_h)$ and $r^*_\Gamma[u_h](z_h)$ denote the adjoint element, interior face and boundary residuals, respectively. Then, the discretization (9) is adjoint consistent if (13) holds also for the exact solutions u and z which is true provided u and z satisfy

$$R^*[u](z) = 0 \ \text{ in } \kappa, \quad r^*[u](z) = 0 \ \text{ on } \partial\kappa \setminus \Gamma, \kappa \in \mathcal{T}_h, \quad r^*_\Gamma[u](z) = 0 \ \text{ on } \Gamma. \tag{14}$$

The adjoint problem and consequently the adjoint consistency of a discretization depends on the specific target functional $J(\cdot)$ under consideration. Given a target functional of the form (7), we see that $R^*[u](z)$ depends on $j_\Omega(\cdot)$, and $r^*_\Gamma[u](z)$ depends on $j_\Gamma(\cdot)$. For obtaining an adjoint consistent discretization, it is in some cases necessary to replace $J(\cdot)$ by a modified target functional $\tilde{J}(\cdot)$ which is consistent if $J(u) = \tilde{J}(u)$ holds for the exact solution u. Furthermore, requiring adjoint consistency may have consequences on the discretization of boundary conditions. In the following we give several examples, see [3].

Linear advection-reaction equation: We consider the linear advection-reaction equation and a compatible target functional of the form:

$$\begin{gathered} \nabla \cdot (\mathbf{b}u) + cu = f \quad \text{in } \Omega, \qquad u = g \quad \text{on } \Gamma_-, \\ J(u) = \int_\Omega j_\Omega \, u \, \mathrm{d}\mathbf{x} + \int_{\Gamma_+} j_\Gamma \, u \, \mathrm{d}s \end{gathered} \tag{15}$$

The discontinuous Galerkin discretization of this problem based on upwind is adjoint consistent and the error $J(u) - J(u_h)$ in the target functional is $\mathcal{O}(h^{2p+1})$ for sufficiently smooth primal and adjoint solutions.

Poisson's equations: We consider the following elliptic model problem and a compatible target functional of the form:

$$
\begin{aligned}
&-\Delta u = f \quad \text{in } \Omega, \qquad u = g_D \quad \text{on } \Gamma_D, \qquad \mathbf{n}\cdot\nabla u = g_N \quad \text{on } \Gamma_N,\\
&J(u) = \int_\Omega j_\Omega\, u \,\mathrm{d}\mathbf{x} + \int_{\Gamma_D} j_D\, \mathbf{n}\cdot\nabla u \,\mathrm{d}s + \int_{\Gamma_N} j_N\, u \,\mathrm{d}s.
\end{aligned} \tag{16}
$$

The non-symmetric interior penalty DG (NIPG) discretization of this problem is adjoint inconsistent and hence the error $J(u) - J(u_h)$ in the target functional is $\mathcal{O}(h^p)$. In contrast to that the error $J(u) - \tilde{J}(u_h)$ of the symmetric version (SIPG) together with following modified target functional, see also [1],

$$
\tilde{J}(u_h) = J(u_h) - \int_{\Gamma_D} \delta(u_h - g_D) j_D \,\mathrm{d}s. \tag{17}
$$

is $\mathcal{O}(h^{2p})$. We note, that without this so-called *IP modification* of $J(\cdot)$ the discretization is adjoint inconsistent and $\mathcal{O}(h^p)$, only. Here, again, all orders of convergence hold provided the primal and adjoint solutions are sufficiently smooth.

The compressible Euler equations: We consider the compressible Euler equations with slip wall boundary conditions and a compatible target functional:

$$
\begin{aligned}
&\nabla\cdot\mathcal{F}^c(\mathbf{u}) = 0 \quad \text{in } \Omega, \qquad \mathbf{v}\cdot\mathbf{n} = 0 \quad \text{on } \Gamma_W,\\
&J(\mathbf{u}) = \int_{\Gamma_W} p(\mathbf{u})\, \mathbf{n}\cdot\boldsymbol{\psi}_{\Gamma_W} \,\mathrm{d}s.
\end{aligned} \tag{18}
$$

Examples of $J(\cdot)$ are the drag and lift coefficient with $\psi_{\Gamma_W} = \frac{1}{C_\infty}\psi$ and $\psi = \psi_d = (\cos(\alpha), \sin(\alpha))^\top$ for the drag and $\psi = \psi_l = (-\sin(\alpha), \cos(\alpha))^\top$ where α is the angle of attack and C_∞ is a constant depending on freestream quantities. DG discretizations of the compressible Euler equations include numerical flux functions $\mathcal{H}(\mathbf{u}_h^+, \mathbf{u}_h^-, \mathbf{n})$ approximating a Riemann problem connecting the states $\mathbf{u}_h^+$ and $\mathbf{u}_h^-$ between neighboring elements. The standard approach of taking the same numerical flux $\mathcal{H}_\Gamma = \mathcal{H}$ on the boundary Γ as in the interior domain and replacing the exterior value $\mathbf{u}_h^-$ by a boundary value function $\mathbf{u}_\Gamma(\mathbf{u}_h^+)$ like in $\int_\Gamma \mathcal{H}_\Gamma(\mathbf{u}_h^+, \mathbf{u}_\Gamma(\mathbf{u}_h^+), \mathbf{n})\mathbf{v}\,\mathrm{d}s$ and computing the target functional like given in (18) is adjoint inconsistent. The adjoint consistency analysis reveals that instead using

$$
\mathcal{H}_\Gamma(\mathbf{u}_h^+, \mathbf{u}_\Gamma(\mathbf{u}_h^+), \mathbf{n}) = \mathbf{n}\cdot\mathcal{F}^c(\mathbf{u}_\Gamma(\mathbf{u}_h^+)), \qquad \text{and} \quad \tilde{J}(\mathbf{u}_h) = J(\mathbf{u}_\Gamma(\mathbf{u}_h^+)), \tag{19}
$$

see also [8], leads to an adjoint consistent discretization.

The compressible Navier-Stokes equations: We consider the compressible Navier-Stokes equations with noslip wall isothermal ($T = T_{\text{wall}}$ on Γ_{iso}) or adiabatic ($\mathbf{n}\cdot\nabla T = 0$ on Γ_{adia}) boundary conditions and a compatible target functional:

$$
\begin{aligned}
&\nabla\cdot(\mathcal{F}^c(\mathbf{u}) - \mathcal{F}^v(\mathbf{u}, \nabla\mathbf{u})) = 0 \quad \text{in } \Omega, \quad \mathbf{v} = (v_1, v_2)^\top = 0 \quad \text{on } \Gamma_W = \Gamma_{\text{iso}} \cup \Gamma_{\text{adia}},\\
&J(\mathbf{u}) = \int_{\Gamma_W} (p\,\mathbf{n} - \underline{\tau}\,\mathbf{n})\cdot\boldsymbol{\psi}_{\Gamma_W} \,\mathrm{d}s.
\end{aligned} \tag{20}
$$

Examples of $J(\cdot)$ are the total (i.e. pressure induced plus viscous) drag or lift coefficient with ψ_{Γ_W} as defined (18). For obtaining an adjoint consistent discretization,

here the boundary terms must be modified analoguous to the boundary terms of the compressible Euler equations. Additionally, if the target functional $J(\cdot)$ in (20) is modified as follows, see [3],

$$\tilde{J}(\mathbf{u}_h) = J(\mathbf{u}_\Gamma(\mathbf{u}_h^+)) + \int_{\Gamma_W} \delta \left(\mathbf{u}_h^+ - \mathbf{u}_\Gamma(\mathbf{u}_h^+)\right) \cdot \mathbf{z}_\Gamma \, \mathrm{d}s \tag{21}$$

where $\mathbf{z}_\Gamma$ is the boundary value of the continous adjoint problem then the discretization is adjoint consistent. This modification corresponds to the IP modification of J for Poisson's equation in (17). If, however, the target functional is evaluated as in (20) then the discretization is adjoint inconsistent.

To summarize: Only in combination with target functionals which are compatible with the primal equations we can expect a DG discretization to be adjoint consistent. It can be shown that only the target functionals given in (15), (16), (18) and (20) are compatible with the respective primal equations and may lead to an adjoint consistent discretization. Additionally, as shown for the compressible Euler and Navier-Stokes equations, special care is required in the discretization of boundary conditions as otherwise adjoint consistency and order doubling is lost.

2. Error estimation and adaptivity: Given a discretization (9) the error $J(u) - J(u_h)$ can be represented by $J(u) - J(u_h) = -\mathcal{N}(u_h, z)$ where z is the exact (and in general unkown) solution to the continuous adjoint problem (8). Replacing z by the solution $\tilde{z}_h \in \tilde{V}_h$ to the discrete adjoint problem (9) we obtain an approximate error representation $J(u) - J(u_h) \approx -\mathcal{N}(u_h, \tilde{z}_h) = \sum_\kappa \eta_\kappa$ which can be decomposed as a sum of local dual-weighted-residual or adjoint-based indicators η_κ. The approximate error representation and the adjoint-based indicators have been successfully applied in the *a posteriori* error estimation and goal-oriented mesh refinement for discontinuous Galerkin discretizations of inviscid and viscous laminar sub-, trans- and supersonic compressible flows, [2, 4, 5, 6], also in combination with anisotropic mesh refinement [7].

References

[1] K. Harriman, D. Gavaghan and E. Süli, *The Importance of adjoint consistency in the approximation of linear functionals using the discontinuous Galerkin finite element method*, Oxford University Computing Laboratory, NA-04/18, (2004).

[2] R. Hartmann, *Adaptive discontinuous Galerkin methods with shock-capturing for the compressible Navier-Stokes equations*, Int. J. Numer. Meth. Fluids **51**(9–10) (2006), 1131–1156.

[3] R. Hartmann, *Adjoint consistency analysis of Discontinuous Galerkin discretizations*, SIAM J. Numer. Anal. (2006), submitted.

[4] R. Hartmann, *Error estimation and adjoint based refinement for an adjoint consistent DG discretization of the compressible Euler equations*, Int. J. Comp. Sci. Math. (2007), to app.

[5] R. Hartmann and P. Houston, *Adaptive Discontinuous Galerkin Finite Element Methods for the Compressible Euler Equations*, J. Comp. Phys. **183** (2002), 508–532.

[6] R. Hartmann and P. Houston, *Symmetric Interior Penalty DG Methods for the Compressible Navier–Stokes Equations II: Goal–Oriented A Posteriori Error Estimation*, Int. J. Num. Anal. Model. **3**(2006), 141–162.

[7] T. Leicht and R. Hartmann, *Anisotropic mesh refinement for discontinuous Galerkin methods in two-dim. aerodynamic flow simulations*, Int. J. Numer. Meth. Fluids (2007), to app.

[8] J. Lu and D. L. Darmofal, *Dual-consistency analysis and error estimation for discontinuous Galerkin discretization: application to first-order conservation laws*, IMA Journal of Numerical Analysis (2006), submitted.

hp–adaptive discontinuous Galerkin FEMs on isotropic and anisotropically refined meshes

Paul Houston
(joint work with Manolis Georgoulis and Edward Hall)

We present an overview of some recent developments concerning the *a posteriori* error analysis and adaptive mesh refinement of non-conforming discontinuous Galerkin (DG) finite element methods for the numerical solution of second-order PDEs with non-negative characteristic form. Here, we shall be particularly concerned with the derivation of *a posteriori* bounds on the error measured in terms of certain output functionals of the solution of practical interest; relevant examples include the lift and drag coefficients for a body immersed into a fluid, the local mean value of the field or its flux through the outflow boundary of the computational domain, and the pointwise evaluation of a component of the solution.

By employing a duality argument we derive so–called weighted or Type I *a posteriori* estimates which bound the error between the true value of the prescribed functional, and the actual computed value. In these error estimates, the element residuals of the computed numerical solution are multiplied by local weights involving the solution of a certain *dual* or *adjoint* problem. On the basis of the resulting *a posteriori* error bound, we design and implement an *hp*–adaptive finite element algorithm to ensure reliable and efficient control of the error in the computed functional with respect to a user–defined tolerance. Here, the adaptive algorithm employed will be based on a combination of local isotropic and anisotropic refinement of the computational mesh and local polynomial degrees. Numerical experiments highlighting the performance of the proposed anisotropic *hp*-adaptive strategy will be presented.

References

[1] E.H. Georgoulis, E. Hall, and P. Houston. *Discontinuous Galerkin Methods for Advection-Diffusion-Reaction Problems on Anisotropically Refined Meshes*, SIAM J. Sci. Comp., (in press).

[2] E.H. Georgoulis, E. Hall, and P. Houston. *Discontinuous Galerkin Methods on hp–Anisotropic Meshes I: A Priori Error Analysis*, Int. J. Comp. Sci. Math., (in press).

[3] E.H. Georgoulis, E. Hall, and P. Houston. *Discontinuous Galerkin Methods on hp–Anisotropic Meshes II: A Posteriori Error Analysis and Adaptivity.* Submitted for publication.

Computational Thermodynamics

Claes Johnson

We present an alternative to Statistical Mechanics as basis of Thermodynamics, based on finite precision computation in the form of stabilized finite element methods for the Euler equations. For more material see the webpage [1].

References

[1] URL: http://www.nada.kth.se/ cgjoh/.

Convergence of an adaptive finite element methods for the p-Laplace equation

Christian Kreuzer
(joint work with Lars Diening)

We report on the recent work [DK07], where we analyze linear convergence of an adaptive finite element mathod for the p-Laplace equation. In particular let Ω be a polyhedral, bounded domain in $\mathbb{R}^d$, $d \in \mathbb{N}$. We consider the following system of nonlinear structure

$$\begin{aligned} -\operatorname{div}(\mathbf{A}(\nabla u)) &= f \qquad \text{in } \Omega, \\ u &= 0 \qquad \text{on } \partial\Omega. \end{aligned} \tag{1}$$

Our considerations include in particular the case of the p-Laplacian, where

$$\mathbf{A}(\nabla u) = (\kappa + |\nabla u|)^{p-2}\, \nabla u, \tag{2}$$

with $1 < p < \infty$, $\kappa \geq 0$, $f \in L^{p'}(\Omega)$, and $\frac{1}{p} + \frac{1}{p'} = 1$.

For computing numerical approximations to the solution of (1) we use a standard adaptive finite element method (AFEM). It consist of the basic loop

$$\text{Solve} \rightarrow \text{Estimate} \rightarrow \text{Mark} \rightarrow \text{Refine} \tag{AFEM}$$

starting from a initial triangulation of Ω. To be more specific, the finite element problem on the current mesh is solved, then the aposteriori error estimator is computed and finally with its help elements are marked for refinement. The marking strategy resorts to *Dörfler's marking* introduced in [Dör96]. The algorithm uses piecewise linear, continuous finite elements, whereas the refinement is realized by newest vertex bisection. This produces a sequence of weak finite element solutions u_k of (1) in nested finite element spaces V_k.

The main result states linear convergence of u_k to the weak solution u of (1). In particular, we show that there exists $\alpha \in (0,1)$, $C > 0$ with

$$\|\mathbf{F}(\nabla u_k) - \mathbf{F}(\nabla u)\|_2^2 + osc_k^2(f) \leq \alpha^{2k} C,$$

where the vector field $\mathbf{F}$ arises from the vector field $\mathbf{A}$ by $\mathbf{F}(\mathbf{a}) := |\mathbf{A}(\mathbf{a})|^{\frac{1}{2}}\, |\mathbf{a}|^{-\frac{1}{2}} \mathbf{a}$. The L^2 norm of the error $\|\mathbf{F}(\nabla u_k) - \mathbf{F}(\nabla u)\|_2^2$ measured in terms of $\mathbf{F}$ is equivalent to the so called *quasi norm* $\|\nabla u_k - \nabla u\|_{(p)}^2$ introduced by Barrett and Liu,

cf. [BL94a]. The *quasi norm* was a breakthrough in the numerical investigation of (1). In particular, Barrett and Liu obtained the best approximation property of the conforming, finite element solution $u_h \in V_h$ in terms of quasi norms, i.e.

$$\|\nabla v - \nabla v_h\|_{(p)}^2 \leq c \min_{\psi_h \in V_h} \|\nabla v - \nabla \psi_h\|_{(p)}^2,$$

In [EL05] it has been proved by Ebmeyer and Liu that for piecewise linear, continuous finite elements and $p > \frac{2d}{d+2}$ the best approximation error can be estimated as

$$\min_{\psi_h \in V_h} \|\nabla v - \nabla \psi_h\|_{(p)}^2 \leq c\, h^2 \int_\Omega (\kappa + |\nabla u|)^{p-2} \, |\nabla^2 u|^2 \, dx. \tag{3}$$

Recently, Diening and Růžička improved these results in [DR06] to the case $p > 1$ admitting also more general finite element spaces. In particular, they showed

$$\|\mathbf{F}(\nabla v) - \mathbf{F}(\nabla v_h)\|_2^2 \leq c \min_{\psi_h \in V_h} \|\mathbf{F}(\nabla v) - \mathbf{F}(\nabla \psi_h)\|_2^2$$

and

$$\|\mathbf{F}(\nabla v) - \mathbf{F}(\nabla \Pi_h v)\|_2^2 \leq c\, h^2 \, \|\nabla \mathbf{F}(\nabla u)\|_2^2, \tag{4}$$

where Π_h is a suitable interpolation operator, e.g. the Scott-Zhang operator. We want to mention that the right hand sides of (3) and (4) are proportional. They express the natural regularity of a *strong* solution of (1) (cf. [Giu03], [BL93a], [ELS05], [Ebm05]).

The technique of quasi-norms founds its way into a posteriori analysis in the work of Liu and Yan [LY01, LY02]. They show that

$$c\, \eta_h^2 - C\, osc_h^2(f) \leq \|\nabla u - \nabla u_h\|_{(p)}^2 \leq C \left(\eta_h^2 + \widetilde{\eta}^2\right)$$

for residual based estimators η_h. Numerical experiments [LY01, CK06] indicate, that these new estimators are indeed sharper and lead to more efficient meshes than existing ones. However for convergence analysis the additional term $\widetilde{\eta}^2$ causes problems, since it forms a gap between the left and the right hand side. In this talk we present estimators that overcome this drawback:

$$c\, \eta_h^2 - C\, osc_h^2(f) \leq \|\mathbf{F}(\nabla u) - \mathbf{F}(\nabla u_h)\|_2^2 \leq C\, \eta_h^2. \tag{5}$$

Recently a posteriori error estimators by gradient recovery have been studied in [CLY06].

Dörfler was the first who proved in [Dör96] linear error reduction of (AFEM) for the linear Laplacian, if the data oscillation is small enough. Later, this additional assumption has been removed by Morin, Nochetto, and Siebert in [MNS00] by additional marking for oscillation. The first convergence result for the nonlinear Laplacian is stated by Veeser [Ve02]. There residual based estimators for the $W^{1,p}$ norm are used. Since there appears a gap in the power between the upper and lower estimates this prevents to prove linear convergence.

The convergence results in the linear case are heavily based on Galerkin orthogonality and the Pythagorean Theorem which yield

$$|||u_h - u|||^2 = |||u_H - u|||^2 - |||u_H - u_h|||^2. \tag{6}$$

in the energy norm. To overcome the lack of orthogonality in the non-linear case we proceed as follows: We show that the energy difference of weak solutions in nested spaces $V_1 \subset V_2$ is proportional to the quasi-norm distance, i.e.

$$\mathcal{J}(u_1) - \mathcal{J}(u_2) \sim \|\nabla u_1 - \nabla u_2\|_{(p)}^2 \sim \|\mathbf{F}(\nabla u_1) - \mathbf{F}(\nabla u_2)\|_2^2,$$

where $\mathcal{J}(u)$ is the energy functional of (1), $u_1 \in V_1$, and $u_2 \in V_2$. This property and the trivial equality

$$\mathcal{J}(u_h) - \mathcal{J}(u) = \big(\mathcal{J}(u_H) - \mathcal{J}(u)\big) - \big(\mathcal{J}(u_H) - \mathcal{J}(u_h)\big)$$

is our substitute for the orthogonality of the error (6).

In the linear, symmetric case it is possible to consider the reduction of the error and the oscillation independently, since the oscillation is solely dependent on the data f. Mekchay and Nochetto showed linear reduction of the sum of error and oscillation for non-symmetric second order linear elliptic PDE in [MN05]. In this case oscillation and error are coupled. A similar effect appears in our non-linear setting. We introduce a new proof for error reduction, which enables us to manage without extra marking for oscillation. Our proof permits to use the fact that oscillation is dominated by the error indicator. Moreover, we show a strict reduction of the difference of energies plus the oscillation in each step.

An essential tool in our calculations in the use of *shifted* N-functions, namely ϕ_a. They are closely related to the quasi-norms, which is best expressed by the relation

$$\big(\mathbf{A}(\mathbf{a}) - \mathbf{A}(\mathbf{b})\big) \cdot (\mathbf{a} - \mathbf{b}) \sim \big|\mathbf{F}(\mathbf{a}) - \mathbf{F}(\mathbf{b})\big|^2 \sim \phi_{|\mathbf{a}|}(|\mathbf{a} - \mathbf{b}|)$$

for $\mathbf{a}, \mathbf{b} \in \mathbb{R}^d$. The shifted N-functions enable us to handle even more general non-linear equations than the p-Laplacian. But most important, the shifted N-functions simplify and clarify the calculations significantly also in the case of the p-Laplacian.

References

[BL93a] J. W. Barrett and W. B. Liu, *Finite element approximation of the p-Laplacian*, Math. Comp. **61** (1993), no. 204, 523–537.

[BL94a] J. W. Barrett and W. B. Liu, *Finite element approximation of degenerate quasilinear elliptic and parabolic problems*, Numerical analysis 1993 (Dundee, 1993), Pitman Res. Notes Math. Ser., vol. 303, Longman Sci. Tech., Harlow, 1994, pp. 1–16.

[BL94b] J.W. Barrett and W.B. Liu, *Finite element approximation of the parabolic p-Laplacian*, Siam J. Numer. Anal. **31** (1994), 413–428.

[CLY06] C. Carstensen and W. B. Liu and N. Yan, *A posteriori FE error control for p-Laplacian by gradient recovery in quasi-norm*, Math. Comput. **75** (1994), no. 256, 1599–1616.

[CK06] C. Carstensen and R. Klose, *A posteriori finite element error control for the p-Laplace problem*, SIAM J. Numer. Anal. **25** (2003), no. 3, 792-814.

[DE05] L. Diening and F. Ettwein, *Fractional estimates for non-differentiable elliptic systems with general growth*, Forum Mathematicum, accepted (2006).

[DK07] L.Diening and C.Kreuzer *Linear convergence of an finite element method for the p-Laplacian equation*, Preprint 03/2007, Mathematisches Institut, Albert-Ludwigs-Universität Freiburg

[DR06] L. Diening and M. Růžička, *Error estimates for interpolation operators in Orlicz-Sobolev spaces and quasi norms*, Preprint, Mathematische Fakultät, Albert-Ludwigs-Universität Freiburg (2006).

[Dör96] W. Dörfler, *A convergent adaptive algorithm for Poisson's equation*, SIAM J. Numer. Anal. **33** (1996), no. 3, 1106–1124.

[Ebm05] C. Ebmeyer, *Gobal regularity in Sobolev spaces for elliptic problems with p-structure on bounded domains*, Trends in partial differential equations of mathematical physics, Progr. Nonlinear Differential Equations Appl., vol. 61, Birkhäuser, Basel, 2005, pp. 81–89.

[EL05] C. Ebmeyer and WB. Liu, *Quasi-norm interpolation error estimates for the piecewise linear finite element approximation of p-Laplacian problems*, Numer. Math. **100** (2005), no. 2, 233–258.

[ELS05] C. Ebmeyer, W. B. Liu, and M. Steinhauer, *Global regularity in fractional order Sobolev spaces for the p-Laplace equation on polyhedral domains*, Z. Anal. Anwendungen **24** (2005), no. 2, 353–374.

[Giu03] E. Giusti, *Direct methods in the calculus of variations*, World Scientific Publishing Co. Inc., River Edge, NJ, 2003.

[LY01] W. Liu and N. Yan, *Quasi-norm local error estimators for p-Laplacian*, SIAM J. Numer. Anal. **39** (2001), no. 1, 100–127 (electronic).

[LY02] ———, *On quasi-norm interpolation error estimation and a posteriori error estimates for p-Laplacian*, SIAM J. Numer. Anal. **40** (2002), no. 5, 1870–1895 (electronic).

[MN05] K. Mekchay and R. H. Nochetto, *Convergence of adaptive finite element methods for general second order linear elliptic PDEs*, SIAM J. Numer. Anal. **43** (2005), no. 5, 1803–1827 (electronic).

[MNS00] P. Morin, R. Nochetto, and K. Siebert, *Data oscillation and convergence of adaptive FEM*, Siam J. Numer. Anal. **38** (2000), 466–488.

[Ve02] A.Veeser, *Convergent adaptive finite elements for the nonlinear Laplacian*, Numer. Math. **92** (2002), no. 4, 743–770.

Adaptive methods for stationary variational problems from a wavelet perspective

Angela Kunoth

When designing adaptive methods for stationary PDEs in variational form, the perhaps mostly used criterion to steer adaptivity is based on controlling the error between the solution and its approximation with respect to some norm. Choosing the energy norm, a corresponding paradigm based on wavelets was developed in a series of papers [4, 5, 6], covering also nonsymmetric and nonlinear elliptic PDEs, see also [7] for a survey. There not only a convergence theory was developed based on perturbation arguments to approximate solutions in infinite-dimensional spaces but, most importantly, also optimal complexity estimates were provided in the following sense: if the solution can be approximated by N terms in a wavelet expansion up to approximation order N^{-s} for some $s > 0$, then the designed schemes recover this approximation with optimal complexity $\mathcal{O}(N)$. The realization of these schemes relies on iterative procedures in infinite-dimensional spaces and a sophisticated approximate matrix-vector multiplication in wavelet coordinates. I presented a variant of these schemes based on inexact conjugate gradient iterations combined with a nested iteration scheme [2, 3].

Moreover, in my talk I discussed an extension of these concepts to optimal control problems with distributed or Neumann boundary control constrained by an elliptic PDE [8], and to problems with Dirichlet boundary control [12]. The corresponding adaptive schemes have been shown to converge, yielding for each of the involved variables (state, costate, control) its own refinement with asymptotical optimal complexity. An important feature of an efficient implementation of these schemes are absolute small uniformly bounded condition numbers of the resulting saddle point matrices [15], see also the survey [11].

Steering adaptivity with respect to some functional of the solution, see [1, 10], the issue of convergence and convergence rates has been studied recently based on finite elements in [13, 14]. Here I have also presented some results on goal-oriented error estimation based on wavelets together with optimal convergence rates and corresponding numerical experiments from [9].

References

[1] R. Becker, R. Rannacher, *An optimal error control approach to a-posteriori error estimation*, Acta Numerica 2001, 1-102.

[2] C. Burstedde, *Fast Optimised Wavelet Methods for Control Problems Constrained by Elliptic PDEs*, Institut für Angewandte Mathematik, Universität Bonn, PhD Dissertation, 2005, `//hss.ulb.uni-bonn.de/diss_online/math_nat_fak/2005/burstedde_carsten`

[3] C. Burstedde, A. Kunoth, *A wavelet-based nested iteration–inexact conjugate gradient algorithm for adaptively solving elliptic PDEs*, Manuscript, July 2007.

[4] A. Cohen, W. Dahmen, R. DeVore, *Adaptive wavelet methods for elliptic operator equations – Convergence rates*, Math. Comp. **70** (2001), 27–75.

[5] A. Cohen, W. Dahmen, R. DeVore, *Adaptive wavelet methods II – Beyond the elliptic case*, Found. Computat. Math. **2** (2002), 203–245.

[6] A. Cohen, W. Dahmen, R. DeVore, *Adaptive wavelet scheme for nonlinear variational problems*, SIAM J. Numer. Anal. **41(5)** (2003), 1785–1823.

[7] W. Dahmen, *Multiscale and wavelet methods for operator equations*, C.I.M.E. Lecture Notes in Mathematics, *Multiscale Problems and Methods in Numerical Simulation*, Springer Lecture Notes in Mathematics, Vol. 1825, Springer-Verlag, Heidelberg, 2003, 31–96.

[8] W. Dahmen, A. Kunoth, *Adaptive wavelet methods for linear–quadratic elliptic control problems: Convergence rates*, SIAM J. Contr. Optim. **43(5)** (2005), 1640–1675.

[9] W. Dahmen, A. Kunoth, J. Vorloeper, *Convergence of adaptive wavelet methods for goal-oriented error estimation*, in: Proceedings of Enumath 2005, 39-60, 2006.

[10] K. Eriksson, D. Estep, P. Hansbo, C. Johnson, *Introduction to adaptive methods for differential equations*, Acta Numerica 1995, 105–158.

[11] A. Kunoth, *Wavelet-based multiresolution methods for stationary PDEs and PDE-constrained control problems*, in: Frontiers in Numerical Analysis, J. Blowey, A. Craig (eds.), Durham 2004, Springer, 2005, 1–63.

[12] A. Kunoth, *Adaptive wavelet schemes for an elliptic control problem with Dirichlet boundary control*, Numer. Algor. **39 (1-3)** (2005), 199–220.

[13] M.S. Mommer, R.P. Stevenson, *A goal oriented adaptive finite element method with convergence rates*, Preprint 1357, Department of Mathematics, Utrecht University, November 2006.

[14] K.-S. Moon, E. v. Schwerin, A. Szepessy, R. Tempone, *Convergece rates of an adaptive dual weighted residual finite element algorithm*, BIT Numerical Mathematics **46** (2006), 367–407.

[15] R. Pabel, *Wavelet Methods for a PDE Constrained Control Problem with Dirichlet Boundary Control*, Institut für Angewandte Mathematik, Universität Bonn, Diploma thesis, 2006.

Fully automatic *hp*-adaptivity for acoustic and electromagnetic scattering in three dimensions

Jason Kurtz
(joint work with Leszek Demkowicz)

We present an algorithm for fully automatic *hp*-adaptivity for finite element approximations of elliptic and Maxwell boundary value problems in three dimensions. The algorithm automatically generates a sequence of coarse grids, and a corresponding sequence of fine grids (obtained by a global *hp*-refinement of the coarse grids), such that the energy norm of the error decreases exponentially with respect to the number of degrees of freedom (d.o.f.) in either sequence. At each step, we employ a discrete optimization algorithm to determine the refinements for the current coarse grid such that the projection-based interpolation error for the current fine grid solution decreases with an optimal rate with respect to the number of d.o.f. added by the refinement. The refinements are restricted only by the requirement that the resulting mesh is at most 1-irregular, but they may be anisotropic in both element size h and order of approximation p.

1. Projection-based interpolation

Our method is based on the theory of conforming *hp* discretizations of the function spaces H^1, $\boldsymbol{H}(\mathrm{curl})$, $\boldsymbol{H}(\mathrm{div})$ and L^2, and the corresponding projection-based interpolation operators [1]. For our present purpose, we only recall the definition of the $\boldsymbol{H}(\mathrm{curl})$ interpolant.

On a hexahedral element K the projection based interpolant $\Pi^{curl}\boldsymbol{E}$ of a function $\boldsymbol{E} \in \boldsymbol{H}^{\epsilon}(\mathrm{curl}, K) \cap \boldsymbol{H}^{1/2+\epsilon}(K)$ is defined in four stages:

$$\begin{aligned} \Pi^{curl}\boldsymbol{E} &= \boldsymbol{E}_0 + \boldsymbol{E}_1 + \boldsymbol{E}_2 + \boldsymbol{E}_3 \\ &\in Q^{p-1,p,p}(K) \times Q^{p,p-1,p}(K) \times Q^{p,p,p-1}(K) \end{aligned}$$

(1) Edge averages: for each edge e, find constant E_0 such that

$$\int_e (E - E_0)_t \, ds = 0$$

(2) Edge projections: find E_1 such that

$$\| \int_0^s (E - E_0 - E_1)_t \|_{0,e} \to \min$$

(3) Face projections: for each face f, find E_2 such that

$$\begin{aligned} &\|\mathrm{curl}_f (E - E_0 - E_1 - E_2)_t\|_{-1/2,f} \to \min \\ &((E - E_0 - E_1 - E_2)_t, \boldsymbol{\nabla}_f \phi)_{-1/2,f} = 0 \quad \forall \phi \in Q^p_{-1}(f) \end{aligned}$$

(4) Interior projection: find E_3 such that

$$\begin{aligned} &\|\boldsymbol{\nabla} \times (\boldsymbol{E} - \boldsymbol{E}_0 - \boldsymbol{E}_1 - \boldsymbol{E}_2 - \boldsymbol{E}_3)\|_{0,K} \to \min \\ &(\boldsymbol{E} - \boldsymbol{E}_0 - \boldsymbol{E}_1 - \boldsymbol{E}_2 - \boldsymbol{E}_3, \boldsymbol{\nabla}\phi)_{0,K} = 0 \quad \forall \phi \in Q^p_{-1}(K) \end{aligned}$$

For the computations below, the fractional face norm is replaced by a weighted L^2-norm.

2. The *hp*-algorithm

The basis of the *hp* algorithm is that we project the fine grid solution separately onto each coarse grid element and onto a nested sequence of meshes that is locally imbedded in the fine grid. For each coarse grid element, this sequence is built dynamically by testing all possible types of local *h*-refinement, and keeping the one that delivers the fastest decay in the projection error with respect to the number of d.o.f. added. By not enforcing the global conformity of the interpolant we obtain a dramatically simplified implementation (compare [2]). The algorithm follows the natural hierarchy in the projection-based interpolation, and so consists of three steps, dealing in turn with edges, faces and element interiors. The optimal refinement from each step provides the minimal refinement (starting point) for the next. The final optimal refinements for elements are then possibly upgraded to maintain 1-irregularity, and applied to the current coarse grid to obtain the next optimal coarse grid, and the whole procedure is repeated.

Here, we only describe the first step, dealing with edges. We use a two-stage discrete optimization algorithm. In stage one, the fine grid solution is projected onto each coarse grid edge, the edge resulting from *p*-enrichment, and a nested sequence of edges resulting from *h*-refinement and built dynamically by enriching the order of the son with largest projection error (the so-called largest son error refinement path). A *local* competition between *p*-enrichment (which adds one local d.o.f.), and the *h*-refinement that also adds one d.o.f., determines the optimal direction (*p* or *h*) of investment for the edge. The decision whether any investment should occur is postponed until stage two.

During stage one, we keep track of the global maximum error decrease rate with respect to the number of local d.o.f. added, relative to the coarse grid, for all refinements tested. In stage two (a *global* competition), all edges that deliver rates within some tolerance (70%) of the global max are flagged for investment, in the optimal direction determined in stage one. If the optimal direction is *h*-refinement, we re-trace the largest son error refinement path until the rate drops below 70% of the global max, possibly adding more than one d.o.f.

The discrete optimization for faces and element interiors is similar to that for edges. For a detailed description of the algorithm and enabling high performance technologies, please see [3].

3. Numerical Example

Consider the electromagnetic scattering from a perfectly electrically conducting (PEC) box in an infinite square PEC waveguide. The box occupies $\Omega_{int} = (1/3, 2/3)^2 \times (-.05, .05)$ and the waveguide $\Omega_\infty = (0,1)^2 \times (-\infty, \infty)$. The frequency ω is midway between the first ($\omega_{10}^c = \omega_{01}^c = \pi$) and second ($\omega_{11}^c = \sqrt{2}\pi$) cutoff frequencies, and we use the incident wave $\boldsymbol{E}^{inc} = \boldsymbol{E}_{10}^{+} = (0, \sin \pi x, 0) e^{-i\beta_{10} z}$, traveling in the $+z$ direction ($\beta_{10} = \sqrt{\omega^2 - \pi^2}$).

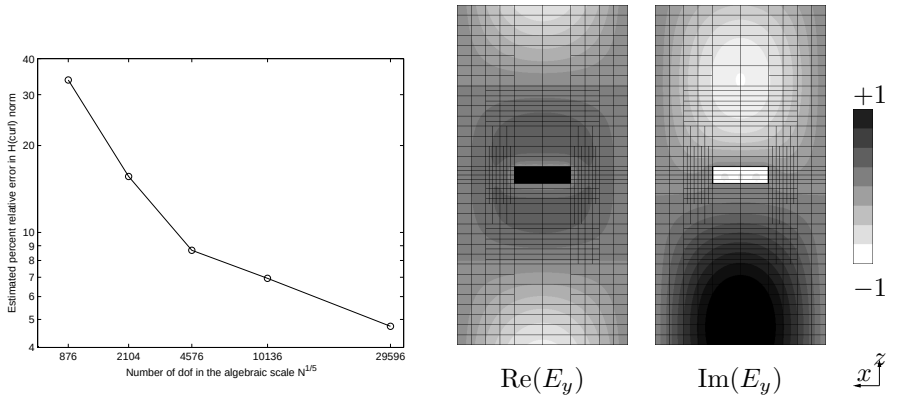


FIGURE 1. Convergence for the sequence of *hp* coarse grids for the waveguide (left) and real and imaginary parts of E_y in the plane $y = 1/2$ (right)

We truncate Ω_∞ with an impedance boundary condition at $z = \pm 1$ (denoted Γ_C) and solve for the scattered electric field $\boldsymbol{E}$ in the truncated exterior domain $\Omega = (0,1)^2 \times (-1,1) \setminus \Omega_{int}$. With Γ_D denoting the lateral walls of the waveguide *and* boundary of Ω_{int}, $\boldsymbol{E}$ satisfies,

$$\begin{aligned} \boldsymbol{\nabla} \times \boldsymbol{\nabla} \times \boldsymbol{E} - \omega^2 \boldsymbol{E} &= 0 \text{ in } \Omega \\ n \times \boldsymbol{E} &= -n \times \boldsymbol{E}^{inc} \text{ on } \Gamma_D \\ n \times \boldsymbol{\nabla} \times \boldsymbol{E} &= i\beta_{10} \boldsymbol{E} \text{ on } \Gamma_C \end{aligned}$$

and the standard variational formulation reads,

$$(1) \quad \left\{ \begin{array}{l} \text{Find } \boldsymbol{E} \in -\boldsymbol{E}^{inc} + \boldsymbol{V} : \\ \displaystyle\int_\Omega \left\{ \boldsymbol{\nabla} \times \boldsymbol{E} \cdot \boldsymbol{\nabla} \times \boldsymbol{F} - \omega^2 \boldsymbol{E} \cdot \boldsymbol{F} \right\} \, dx + i\beta_{10} \int_{\Gamma_C} \boldsymbol{E} \cdot \boldsymbol{F} \, d\Gamma = 0 \quad \forall \boldsymbol{F} \in \boldsymbol{V} \end{array} \right.$$

where $\boldsymbol{V} = \{ \boldsymbol{F} \in \boldsymbol{H}(curl, \Omega) \ : \ n \times \boldsymbol{F} = 0 \text{ on } \Gamma_D \}$.

From an initial coarse grid with 26 elements and $p = 2$, we were able to execute five steps of *hp* adaptive refinement, with the estimated percent relative error for the sequence of coarse grids shown in Figure 1 (left). The convergence is exponential, with a *steeper* pre-asymptotic rate. Real and imaginary parts of E_y from the final fine grid (653K dof) are shown in Figure 1 (right). Cross sections of the final coarse grid orders along the y-axis are shown in Figure 2.

REFERENCES

[1] L. Demkowicz and A. Buffa, H^1, $\boldsymbol{H}$(curl) *and* $\boldsymbol{H}$(div)*-conforming projection-based interpolation in three dimensions. Quasi-optimal p-interpolation estimates*, Comput. Methods Appl. Mech. Engrg. **194** (2005), 267–296.

[2] W. Rachowicz, D. Pardo and L. Demkowicz, *Fully automatic hp-adaptivity in three dimensions*, Comput. Methods Appl. Mech. Engrg. **195** (2006), 4816–4842.

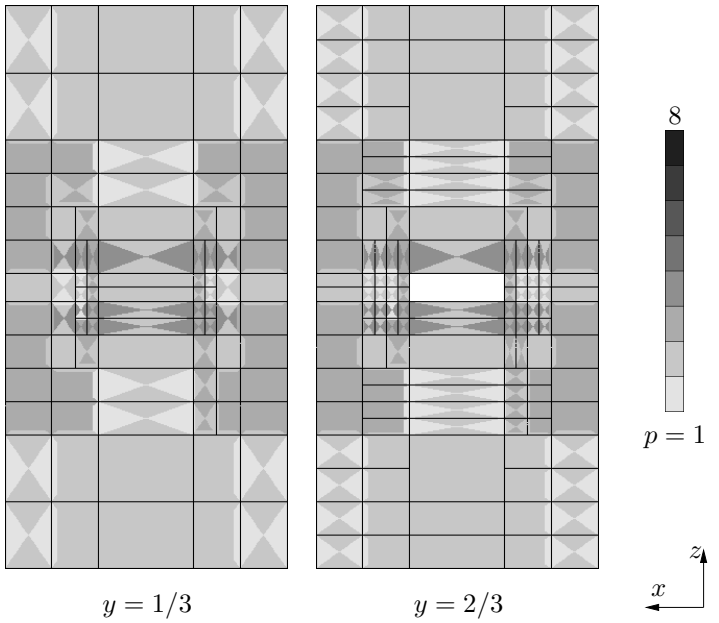


FIGURE 2. Cross sections of the final coarse grid in the planes $y = 1/3$ (left) and $y = 2/3$ (right) viewed from the $+y$ direction.

[3] J. Kurtz, Fully Automatic *hp*-Adaptivity for Acoustic and Electromagnetic Scattering in Three Dimensions, Ph.D. Thesis, The University of Texas at Austin, May 2007.

On global error control for parabolic PDEs

Jens Lang
(joint work with Kristian Debrabant and Jan Verwer)

Let us first suppose that we are given the initial value problem for the system of ODEs in $\mathbb{R}^m$

$$w' = F(t,w)\,, \quad w(0) = w_0\,, \qquad 0 < t \le T\,, \tag{1}$$

and a sequence of approximations $v(t_n)$ to its exact solution values $w(t_n)$ computed by a numerical integration method at a certain time grid

$$0 = t_0 < t_1 < \cdots < t_n < \cdots < t_{N-1} < t_N = T\,. \tag{2}$$

Hereby the major research concerns are efficiency: how to get the $v(t_n)$ at minimal CPU costs (if $m \gg 1$), and reliability: how large is the global error

$$e(t) = v(t) - w(t), \tag{3}$$

where $v(t)$ is calculated by a suitable interpolation method provided by the integrator.

Existing popular codes focus on efficiency by adaptively optimizing time grids (2) in accordance with local error control. Such a control makes sense if solutions exhibit sharp changes at local intervals much smaller than the total interval $[0,T]$ and are smooth elsewhere. However, local errors (errors made within a single integration step) may substantially differ from the global ones (3). This largely depends on the conditioning (stability) of the system (1) at hand (sensitivity to growth in time of perturbations of w_0 and $F(t,w)$). If a system is well-conditioned, a well designed local error control [5, 6] will work out reliably. But if the conditioning is bad, even the best designed local error control should not be trusted.

For global error control it is necessary to take into account the conditioning of system (1). Herewith it is desirable to avoid strict a priori error bounds as these can be overly pessimistic, e.g. when fortunate cancellation effects occur. Taking into account the conditioning of system (1) is best done during actual computation. This requires at least two full integrations over $[0,T]$, both in the classical (forward-forward) approach [7] based on the first variational equation and the adjoint (forward-backward) approach based on the adjoint method combined with a small sample statistical initialization [1]. Numerical experiments in [4] for ODE systems have shown, using the 3rd-order, A-stable Runge-Kutta-Rosenbrock method ROS3P as example integrator, that classical global error estimation is remarkably reliable.

With the residual error defined by

$$r(t) = v'(t) - F(t,v(t)),$$

the global error fulfills the initial value problem

$$e'(t) \;=\; F(t,v(t)) - F(t,w(t)) + r(t), \quad 0 < t \le T, \qquad e(0) = 0.$$

The mean value theorem for vector functions yields

$$e'(t) = F'(t, v(t))e(t) + r(t) + \mathcal{O}(e(t)^2). \tag{4}$$

Apparently, by implementing a proper choice of the defect $r(t)$ solving this equation will in leading order provide approximations to the true global error. To do so, we define $v(t)$ by piecewise cubic Hermite interpolation. By Taylor expansion one can show that the cubic Hermite defect halfway the step interval can be used to retrieve in leading order the local error of any one step method of order $1 \le p \le 3$.

Following the arguments given in [4], Section 2.1, we consider instead of (4) the step size frozen version

$$\begin{aligned} e'(t) &= F'(t_n, v(t_n))\, e(t) + \tfrac{2}{3} r(t_{n+\frac{1}{2}}),\ t \in (t_n, t_{n+1}],\ n = 0, \ldots, N-1, \\ e(0) &= 0 \end{aligned}$$

to approximate the global error $e(t)$. In addition, working for the local error with

$$Est = \frac{2}{3} \left(I - \gamma \tau_n F'(t_n, v(t_n))\right)^{-1} r(t_{n+1/2}) \,,$$

where γ is the stability coefficient of ROS3P, the property of tolerance proportionality [5] is asymptotically ensured, that is, there exists a linear relationship between the global error and the local accuracy tolerance. Thus, $e(t)$ can be successfully controlled by a second run with an adjusted local tolerance.

This approach can be extended to parabolic initial boundary value problems

$$\partial_t u(t,x) = f(t, x, u(t,x), \partial_x u(t,x), \partial_{xx} u(t,x)) \,, \quad t \in (0,T] \,,\ x \in \Omega \subset \mathbb{R}^d \,,$$

with appropriate initial and boundary conditions. Application of the Method of Lines on a spatial mesh Ω_h, $h > 0$, gives

$$\begin{aligned} M_h\, U_h'(t) &= F_h(t, U_h(t)) \,, \qquad t \in (0,T] \,, \\ U_h(0) &= U_{h,0} \,, \end{aligned} \tag{5}$$

Let $R_h : u(t, \cdot) \to R_h u(t)$ be the restriction operator which maps $u(t)$ to its spatial degrees of freedom. Defining the spatial discretization error by

$$\eta_h(t) = U_h(t) - R_h u(t) \,,$$

the vector of overall global errors $E_h(t) = V_h(t) - R_h u(t)$ may be written as sum of the global time and spatial error, that is,

$$E_h(t) = e_h(t) + \eta_h(t) \,.$$

Since the global time error can be controlled as in the ODE case, it remains to estimate the global spatial error. By making use of the restriction operator R_h, the spatial truncation error is defined by

$$\alpha_h(t) = M_h \left(R_h u\right)'(t) - F_h(t, R_h u(t)) \,. \tag{6}$$

From (5) and (6), it follows that the global spatial error $\eta_h(t)$ representing the accumulation of the spatial discretization error, is the solution of the initial value

problem

$$\begin{aligned} M_h\,\eta_h'(t) &= F_h(t,U_h(t)) - F_h(t,R_h u(t)) - \alpha_h(t)\,, \qquad t\in(0,T]\,,\\ \eta_h(0) &= 0 \end{aligned}$$

where we have used $U_{h,0} = R_h u_0$, which bears no restriction. Again, the mean value theorem for vector functions yields

$$\begin{aligned} M_h\,\eta_h'(t) &= \partial_{U_h} F_h(t,U_h(t))\,\eta_h(t) - \alpha_h(t) + \mathcal{O}(\eta_h(t)^2), \qquad t\in(0,T],\\ \eta_h(0) &= 0\,. \end{aligned}$$

Apparently, implementing a proper choice of $\alpha_h(t)$ will in leading order provide approximations of the global spatial error. To estimate $\alpha_h(t)$ by Richardson extrapolation [2], we consider a second semi-discretization on Ω_{2h}

$$M_{2h}U_{2h}'(t) = F_{2h}(t,U_{2h}(t))$$

and assume that $\eta_h(t)$ is of order q with respect to h. Then by Taylor expansion we obtain

$$\alpha_{2h}(t) = \frac{2^q}{2^q-1}\Big(M_{2h}(V_h^c)'(t) - F_{2h}(t,V_h^c(t))\Big) + \mathcal{O}(\tau^p) + \mathcal{O}(h^{q+1}),$$

where $V_h^c(t)$ is the vector $V_h(t)$ restricted to the coarser grid Ω_{2h}. Finally, an approximation $\tilde\alpha_h(t)$ of the spatial truncation error on the (original) fine mesh is obtained by interpolation respecting the order of accuracy, which serves to compute an estimate of $\eta_h(t)$. The control of $\eta_h(t)$ is obtained through (uniform) mesh refinement.

Based on the control of both the global spatial and global time error, one can now use an adequate control strategy to balance them in order to achieve an accuracy imposed by the user. Our numerical examples confirm the reliability of the estimation and control strategies [3].

References

[1] Y. Cao, L. Petzold, *A posteriori error estimation and global error control for ordinary differential equations by the adjoint method*, SIAM J. Sci. Comput. **26** (2004), pp. 359-374.

[2] M. Berzins, *Global error estimation in the method of lines for parabolic equations*, SIAM J. Sci. Stat. Comput. **9** (1988), pp. 687-703.

[3] K. Debrabant, J. Lang, *On global error estimation and control for parabolic equations*, Preprint No. 2512, Technische Universität Darmstadt, Fachbereich Mathematik (2007), submitted.

[4] J. Lang, J. G. Verwer, *On global error estimation and control for initial value problems*, SIAM J. Sci. Comput. **29** No. 4 (2007), 1460–1475.

[5] L.F. Shampine, *Numerical Solution of Ordinary Differential Equations*, Chapman & Hall (1994), New York.

[6] L.F. Shampine, *Error estimation and control for ODEs*, J. Sci. Comput. **25** No. 1 (2005), 3–16.

[7] P.E. Zadunaisky, *On the estimation of errors propagated in the numerical integration of ordinary differential equations*, Numer. Math. **27** (1976), pp. 21-39.

A basic convergence result for conforming adaptive finite element methods

Pedro Morin
(joint work with Kunibert G. Siebert and Andreas Veeser)

A quite popular, natural adaptive version of classical finite element methods consists of the loop

$$\text{SOLVE} \to \text{ESTIMATE} \to \text{MARK} \to \text{REFINE}, \tag{1}$$

that is: solve for the finite element solution on the current grid, compute the a posteriori error estimator, mark with its help elements to be subdivided, and refine the current grid into a new, finer one. While there is a rather elaborated theory for the derivation of a posteriori error estimators, see e.g. [1, 3, 18], the theoretical understanding of the convergence and complexity of such methods is in the early stages.

Babuška/Vogelius [2] give an analysis of (1) for linear, elliptic, and symmetric problems in 1d. The first multidimensional result is Dörfler [8]. It ensures with pathbreaking ideas that, after a pre-adaptation to data, (1) reduces the error below any prescribed tolerance. Proper convergence without conditions on the initial grid was proved by Morin/ Nochetto/Siebert [10]. The latter work was generalized in various directions by, e.g., [5, 6, 7, 9, 11, 14, 15, 17]. Relying on techniques from Binev/Dahmen/DeVore [4] and new ideas, Stevenson [16] gives an important complexity result for an algorithm that is quite close to (1).

Without any doubts, these results are an important progress in the theoretical understanding of (1). Nevertheless, a critical review reveals the following limitations:

- *Symmetric elliptic problems.* Except for [6, 9], all aforementioned results are within a coercive elliptic variational framework. Carstensen/Hoppe [6] treat a mixed formulation for the Poisson problem by exploiting a close relationship to the direct discretization with Crouzeix-Raviart elements. Mekchay/Nochetto [9] allow for a non-symmetric operator, at the price that the initial grid has to be sufficiently fine – a condition of a priori spirit, the necessity of which is not supported by numerical experiments even for convection-dominated diffusion problems.
- *Conforming discretizations and Galerkin solutions.* In all results the discrete space(s) are included in the continuous one(s) and the discrete solution is the Galerkin approximation.
- *Dörfler's strategy and special marking for oscillation.* Except for [14], all convergence and complexity results assume Dörfler's strategy. However, numerical results strongly suggest that, for instance, the maximum strategy is competitive with Dörfler's. Results with the standard residual error estimator require a special treatment like marking or pre-adaptation for (data) oscillation, although the standard residual estimator dominates

oscillation and algorithms without special treatment of oscillation also converge.

- *Artificial conditions for refinement.* All results require a certain, non-minimal subdivision depth for patches associated with marked elements, e.g., the creation of interior nodes is often required. Computational evidence does not support the necessity of these requirements for convergence or quasi-optimal complexity. In addition, such requirements complicate the implementation and, if the required subdivision depth is quite big, yield (1) non-practical.

We presented a new, basic convergence result for (1) applied to linear boundary value problems. The convergence result holds for very general assumptions that are fulfilled by most of the problems analyzed in practice. These assumptions involve the problem itself, the refinement framework, the finite element spaces, the approximate solution, the a posteriori error estimator, the marking strategy and the step REFINE. They ensure the convergence in the following sense:

Let u be the exact solution and let $\|\cdot\|$ be the norm of the trial space. For each iteration k, denote the approximate solution by u_k and the a posteriori error estimator by $\mathcal{E}_k$. Then both error and estimator converge to 0*:*

$$\|u_k - u\| \to 0 \quad \text{and} \quad \mathcal{E}_k \to 0 \quad \text{as} \quad k \to \infty. \tag{2}$$

Our assumptions are sufficiently general and applicable to a wide variety of problems, they hold in particular for:

- Saddle point problems, non-symmetric problems without assuming a sufficiently fine initial grid;
- various types of a posteriori error estimators, including the ZZ one and estimators where the (discrete) lower bound requires a very fine, local extension of the finite element trial space;
- the maximum and equidistribution strategy, without extra marking for oscillation;
- a minimal rule for REFINE, which does not necessarily entail the creation of interior nodes.

Our proof differs from the aforementioned ones in the following aspects:

- *Without strict error reduction and without extra regularity.* Except for [14], all previous convergence proofs for linear problems use a quasi-orthogonality result to prove the following: if oscillation is relatively small, then one iteration of (1) provides a uniformly strict error reduction. To compensate for the missing quasi-orthogonality result for nonlinear potential operators, Siebert/Veeser [15] and Veeser [17] control the residual by the energy reduction in one iteration of (1) and then exploit the fact that the energy reduction vanishes in the limit. Here, we use a similar argument that covers also non-potential operators which neither assumes nor implies regularity of the exact solution beyond the trial space.

- *Estimator convergence first.* With the strict error reduction, convergence of error and estimator are shown simultaneously. Here and in [14, 15, 17], the convergence of the estimator is first derived by exploiting the (discrete) local lower but not the upper bound. The upper bound is then used to obtain the convergence of the error.
- *Without residual control in one iteration.* The strict error reduction and the residual control by the energy reduction share the following features: they involve two successive approximate solutions and they split the estimator into marked and non-marked indicators. These features entail the aforementioned artificial conditions for refinement. Here we avoid this by means of a new splitting of the estimator, and a local lower bound for the difference of a discrete solution and one limiting solution that is known to exist.

Since the strict error reduction is used in the complexity result [16], one may consider its absence as a disadvantage. On the other hand, for solutions of non-coercive problems with, e.g., layers, such a result appears to be unrealistic when starting from a coarse initial grid.

Two corollaries can be deduced from this result, which can be found in detail in [13]. The first one provides necessary and sufficient conditions on marking for (2), while the second gives such a condition for reaching any prescribed tolerance in a finite number of iterations. Another corollary from the convergence proof, namely the convergence of algorithms adapting for a (semi)norm that is weaker than the one of trial space, is given in [12].

References

[1] M. Ainsworth, J. T. Oden, *A posteriori error estimation in finite element analysis*, Wiley-Interscience, New York, 2000.

[2] I. Babuška, M. Vogelius, *Feedback and adaptive finite element solution of one-dimensional boundary value problems*, Numer. Math. 44 (1984), 75-102.

[3] I. Babuška, T. Strouboulis, *The finite element method and its reliability*, The Clarendon Press Oxford University Press, New York, 2001.

[4] P. Binev, W. Dahmen, R. DeVore, *Adaptive finite element methods with convergence rates*, Numer. Math. 97 (2004), 219–268.

[5] J. M. Cascón, R. H. Nochetto, K. G. Siebert, *Design and convergence of AFEM in H(div)*, Preprint Augsburg 2006.

[6] C. Carstensen, R. H. W. Hoppe, *Error reduction and convergence for an adaptive mixed finite element method*, Math. Comp. 75 (2006), 1033–1042.

[7] Z. Chen, J. Feng, *An adaptive finite element algorithm with reliable and efficient error control for linear parabolic problems*, Math. Comp. 73 (2004), 1167–1193.

[8] W. Dörfler, *A convergent adaptive algorithm for Poisson's equation*, SIAM J. Numer. Anal. 33 (1996), 1106–1124.

[9] K. Mekchay, R. H. Nochetto, *Convergence of adaptive finite element methods for general second order linear elliptic PDE*, SIAM J. Numer. Anal. 43 (2005), 1803–1827.

[10] P. Morin, R. H. Nochetto, K. G. Siebert, *Data oscillation and convergence of adaptive FEM*, SIAM J. Numer. Anal. 38 (2000), 466–488.

[11] P. Morin, R. H. Nochetto, K. G. Siebert, *Local problems on stars: a posteriori error estimators, convergence, and performance*, Math. Comp. 72 (2003), 1067–1097.

[12] P. Morin, K. G. Siebert, A. Veeser, *Convergence of finite elements adapted for weak norms*, Preprint 2/2007, Dipartimento di Matematica "F. Enriques", Università degli Studi di Milano.
[13] P. Morin, K. G. Siebert, A. Veeser, *A Basic Convergence Result for Conforming Adaptive Finite Elements*, Preprint 1/2007, Dipartimento di Matematica "F. Enriques", Università degli Studi di Milano.
[14] K. G. Siebert, A. Veeser, *Convergence of the equidistribution strategy*, Oberwolfach Reports 2 (2005), 2129–2131.
[15] K. G. Siebert, A. Veeser, *A unilaterally constrained quadratic minimization with adaptive finite elements*, to appear in SIAM J. Optim.
[16] R. Stevenson, *Optimality of a standard adaptive finite element method*, Preprint No. 1329, 23 pages, Department of Mathematics, Utrecht University. May 2005.
[17] A. Veeser, *Convergent adaptive finite elements for the nonlinear Laplacian*, Numer. Math. 92 (2002), 743-770.
[18] R. Verfürth, *A review of a posteriori error estimation and adaptive mesh-refinement techniques*, Adv. Numer. Math., John Wiley, Chichester, UK, 1996.

Optimal multilevel methods on graded bisection grids

Ricardo H. Nochetto
(joint work with Long Chen and Jinchao Xu)

Adaptive finite element methods (AFEM) are now widely used in scientific and engineering computation to optimize the relation between accuracy and degrees of freedom. They use a posteriori error estimators to gather information about the approximation quality and lead to highly graded meshes that are far from quasiuniform.. This talk deals with the optimal solution of the resulting linear algebraic systems by multilevel methods.

We design additive BPX-type preconditioners and multiplicative V-cycle multigrid methods on graded bisection grids. Early work on the convergence analysis of multigrid methods relies on two rather restrictive regularity assumptions [3]. The first one is an H^2-regularity assumption on the solution of elliptic equations. The second assumption is on the grid geometry: the underlying grids are obtained by uniform refinement from an initial grid. These two regularity assumptions do not hold in applications of AFEM.

We use the framework of subspace correction methods developed by J. Xu [6] to remove the H^2-regularity assumption of the solution and a novel decomposition of bisection grids to remove the quasi-uniform assumption on the grids.

The existing analysis of adaptive multilevel methods relies on some restrictive assumptions on the refinement region. For instance, the adaptive grids considered by Bramble el al in [1] are defined in terms of a given sequence of nested subdomains

$$\Omega_J \subseteq \Omega_{J-1} \subseteq \cdots \subseteq \Omega_0 = \Omega. \tag{1}$$

The grid of Ω_k is obtained by refining elements of Ω_{k-1} that belong to the region Ω_k; this is called nested refinement. It implies that if an element τ is not refined in k-th level, then it cannot be refined afterwards. The assumption (1), unfortunately, does not hold for practical AFEM using *a posteriori* error estimates because a

coarse element can be subsequently refined after very fine elements are added around the singularity region.

Wu and Chen [5] have recently given a refined analysis of adaptive multigrid methods on grids obtained by the newest vertex bisection in two dimensions. Their analysis uses a complicated geometric structure of bisection grids and thus its generalization to three or higher dimensions seems difficult.

Our algorithm and analysis are based on a novel decomposition of bisection grids which are essentially different from [5] and other existing mutlilevel methods on adaptive grids. Roughly speaking, for any triangulation $\mathcal{T}_N$ obtained by a suitable bisection method from an initial triangulation $\mathcal{T}_0$, we write

$$\mathcal{T}_N = \mathcal{T}_0 + \mathcal{B}, \tag{2}$$

where $\mathcal{B} = \{b_1, b_2, \cdots, b_N\}$ denotes N compatible bisections. Each bisection b_i is restricted to a small region ω_i with quasi-uniform meshsize and its application preserves mesh conformity. This decomposition serves as a general bridge to transfer results from quasi-uniform grids to graded bisection grids. In particular, our main contributions are as follows:

(1) We provide a unified analysis for any spatial dimensions; in particular, we prove uniform convergence of V-cycle multigrid for H^1 systems on bisection grids in three dimensions.
(2) Our methods suggest a new way to implement multilevel methods by finding the decomposition of bisection grids via coarsening from the finer mesh [2].
(3) We present our analysis in a general framework that extends to other problems; in fact we comment on the design and analysis of adaptive multigrid methods for the $H(\mathrm{curl})$ and $H(\mathrm{div})$ systems in three dimensions.

We now briefly present our approach. Let $\Omega \subset \mathbb{R}^d, d \geq 2$ be a polyhedral domain and $a(u,v) := \int_\Omega \nabla u \cdot \nabla v$. Given a triangulation $\mathcal{T}$ of Ω, we choose a linear finite element space $\mathbb{V}(\mathcal{T}) \subset H_0^1(\Omega)$ and consider the finite element approximation $u \in \mathbb{V}(\mathcal{T})$ of the second order elliptic equations

$$a(u,v) = \langle f, v\rangle, \quad \forall v \in \mathbb{V}(\mathcal{T}). \tag{3}$$

where $f \in H^{-1}(\Omega)$ and $\langle \cdot, \cdot \rangle$ is the usual duality pairing. For simplicity, we assume that Ω is triangulated exactly and the triangulation $\mathcal{T}$ of Ω is shape regular and conforming. However, we do not impose that $\mathcal{T}$ is quasi-uniform since $\mathcal{T}$ is obtained through bisection methods and could thus be highly non-uniform.

On the basis of the novel decomposition (2) of bisection grids, we give a multilevel space decomposition for finite element spaces $\mathbb{V} = \mathbb{V}(\mathcal{T}_N)$. We let $\mathbb{V}_0 = \mathbb{V}(\mathcal{T}_0)$ and, for each compatible bisection b_i with $i = 1, \cdots, N$, we define a local space $\mathbb{V}_i \subset \mathbb{V}$. We then have a space decomposition

$$\mathbb{V} = \sum_{i=0}^{N} \mathbb{V}_i. \tag{4}$$

We prove the following two key properties for the space decomposition (4):

- For any $v \in \mathbb{V}$, there exist $v_i \in \mathbb{V}_i, i = 0, \cdots, N$ such that $v = \sum_{i=0}^{N} v_i$ and

$$\sum_{i=0}^{N} h_i^{-2} \|v_i\|^2 \lesssim |v|_1^2. \tag{5}$$

- For any $u_i, v_i \in \mathbb{V}_i, i = 0, \cdots, N$, we have

$$\Big| \sum_{i=1}^{N} \sum_{j=i+1}^{N} (u_i, v_j)_1 \Big| \lesssim \left(\sum_{i=1}^{N} |u_i|_1^2 \right)^{1/2} \left(\sum_{i=1}^{N} h_i^{-2} \|v_i\|^2 \right)^{1/2}. \tag{6}$$

With the help of (5) and (6), we are able to obtain optimal multilevel methods including BPX preconditioner and V-cycle multigrid methods for solving algebraic systems arising from (3) on graded bisection grids. In addition, we use these results in conjunction with the relation between $H^1(\Omega)$, $H(\mathrm{curl}; \Omega)$ and $H(\mathrm{div}; \Omega)$, along with regular decomposition of functions in these spaces, to extend the multilevel methods recently proposed by Hiptmair and Xu [4] for $H(\mathrm{curl}; \Omega)$ and $H(\mathrm{div}; \Omega)$ to graded bisection grids.

References

[1] J. H. Bramble, J. E. Pasciak, J. Wang, and J. Xu. Convergence estimates for product iterative methods with applications to domain decomposition. *Mathematics of Computation*, 57:1–21, 1991.

[2] L. Chen and C.-S. Zhang. A coarsening algorithm and multilevel methods on adaptive grids by newest vertex bisection. Technical report, Submitted, 2007.

[3] W. Hackbusch. *Multigrid Methods and Applications*, volume 4 of *Computational Mathematics*. Springer–Verlag, Berlin, 1985.

[4] R. Hiptmair and J. Xu. Nodal auxiliary space decomposition in $H(\mathrm{curl}; \Omega)$ and $H(\mathrm{div}; \Omega)$, Research report no 2006-9, ETH Zurich, Switzerland, 2006.

[5] H. Wu and Z. Chen. Uniform convergence of multigrid v-cycle on adaptively refined finite element meshes for second order elliptic problems. *Science in China: Series A Mathematics*, 49(1):1–28, 2006.

[6] J. Xu. Iterative methods by space decomposition and subspace correction. *SIAM Review*, 34:581–613, 1992.

A posteriori existence in numerical computations

Christoph Ortner

Let X, Y be Banach spaces and let $F : X \to Y$ be Fréchet differentiable. We wish to solve the nonlinear equation $F(u) = 0$. A point u of the domain of definition of F is called regular if $F'(u)$ is an isomorphism, i.e., $F'(u)^{-1}$ is a bounded linear operator (see [1, Proposition 2.1]). A posteriori error estimates for non-monotone nonlinear problems are typically formulated in the following way (see e.g. [1, Proposition 2.1]): *If u is a regular solution to $F(u) = 0$ and U is a numerical solution which is sufficiently close to u then* $\|u - U\|_X \leq c\|F(U)\|_Y \|F'(u)^{-1}\|_{L(Y,X)}$.

In this talk, I develop the following simple observation: the approximation U, which we may have computed numerically, solves the equation $G(U) = 0$, where

$G(v) = F(v) - F(U)$. Thus, by reversing the role of approximate and exact solution, we see that a solution u satisfying $F(u) = 0$ could be considered the approximate solution to the new problem $G(U) = 0$ and its residual is again $\|F(U)\|_Y$. In contrast to the previous situation, however, we now need to assume that U is regular rather than a 'nearby exact solution' u which we often do not know to exist. More precisely, we shall prove that, *if a regular point $U \in X$ has a sufficiently small residual $\|F(U)\|_Y$ then there exists a nearby exact solution u to the equation $F(u) = 0$ such that $\|u - U\|_X \le c\|F(U)\|_Y \|F'(U)^{-1}\|_{L(Y,X)}$.*

In the abstract Banach space setting, I present the following result, which simply requires a tracking of the constants in a suitably chosen proof of the Inverse Function Theorem.

Theorem. *Suppose that $U \in X$ is a regular point and that F is Fréchet differentiable in a sufficiently large neighbourhood of U. Let $\sigma \ge \|F'(U)^{-1}\|$, let $\eta \ge \|F(U)\|_Y$, and let L be an upper bound for the Lipschitz constant of F' in $B(U, R)$, where $R = 2\eta\sigma$. If, in addition, the* a posteriori existence condition

$$2\sigma^2\eta L < 1 \tag{1}$$

is satisfied, then there exists a unique $u \in B(U, R)$ such that $F(u) = 0$. Furthermore, we have the error estimate

$$\|u - U\|_X \le 2\sigma\eta. \tag{2}$$

I then proceed by showing the applicability of the idea at the nonlinear Laplace equation

$$-\Delta u + f(x, u) = 0 \text{ in } \Omega, \quad u = 0 \text{ on } \partial\Omega,$$

which is posed in its weak form, setting $X = H_0^1(\Omega)$, $Y = H^{-1}(\Omega)$ and

$$\langle F(u), \varphi\rangle = \int_\Omega \nabla u \cdot \nabla\varphi + f(x, u)\varphi \,\mathrm{d}x. \tag{3}$$

Under suitable growth hypotheses on f, and assuming that f_u is globally Lipschitz continuous, F is well-defined and differentiable and, moreover, F' is globally Lipschitz continuous.

Let $S_0^k(\mathcal{T}) \subset H_0^1(\Omega)$ be a Lagrange finite element space over a tetrahedral mesh $\mathcal{T}$, and let $U \in S_0^k(\mathcal{T})$ be the corresponding finite element Galerkin approximation to (3). In order to apply the above theorem, we need to estimate the residual and the stability of the linearized equation. The estimation of the residual $\|F(u)\|_{H^{-1}}$ is standard,

$$\|F(u)\|_{H^{-1}}^2 \le \eta = C \sum_{T\in\mathcal{T}} \Big(h_T^2 \| - \Delta U + f(x, U)\|_{L^2(T)}^2 + h_T \|[\nabla U]\|_{L^2(\partial T\setminus\partial\Omega)}^2 \Big),$$

where C depends only on the mesh quality and h_T is a measure of the local mesh size.

The stability constant $\|F'(U)^{-1}\|$, on the other hand, can be computed using an eigenvalue estimate. Namely, it holds that $\|F'(U)^{-1}\| = 1/\lambda$, where λ is the

smallest H_0^1 eigenvalue of $F'(U)$, i.e.,

$$\lambda = \inf_{\varphi\in H_0^1, \|\nabla\varphi\|_{L^2}=1} \int_\Omega \Big[|\nabla\varphi|^2 + f_u(x,U)\varphi^2\Big]\,\mathrm{dx}.$$

This eigenvalue may be estimated via

$$\Lambda = \inf_{\Phi\in H_0^1, \|\nabla\Phi\|_{L^2}=1} \int_\Omega \Big[|\nabla\Phi|^2 + f_u(x,U)\Phi^2\Big]\,\mathrm{dx}.$$

If Ω is convex, then it can be shown that, either $\lambda \geq 1/2$, or

$$\lambda \geq \Lambda - C(1+\Lambda)\|f_u(x,U)\|_{L^\infty}^2 h_{\mathcal{T}}^2,$$

where $h_{\mathcal{T}}$ is the global mesh size and C depends only on the mesh quality and the diameter of Ω. Generalizations to non-convex domains are in principle straightforward but the determination of the constants is more difficult in that case.

Using these constructions we can (up to round-off errors) rigorously justify the existence of exact solutions near a computed Galerkin approximation. Some numerical examples are given that demonstrate further practical aspects of the approach. An earlier version of these results, as well as an application to an interesting quasilinear problem in one dimension, can be found in [2].

With somewhat different aims, the ideas presented in this talk have been developed previously for weak as well as strong solutions of the nonlinear Laplace equation in convex and non-convex domains. For a fairly recent overview article see [3]. For dynamical systems similar ideas can also be employed (see for example [4]). I thank Willy Dörfler, Mats Larson and Stig Larssen for pointing me to the relevant literature.

References

[1] R. Verfürth, *A Review of A Posteriori Error Estimation and Adaptive Mesh-Refinement Techniques*, John Wiley & Sons Ltd. (1996)

[2] C. Ortner, *A posteriori existence in numerical computations*, IMATI-CNR Pavia, Report No. **1-22** (2006)

[3] M. Plum, *Computer-assisted enclosure methods for elliptic differential equations*, Linear Algebra and its Approximations **324** (2001), 147–187

[4] B.A. Coomes, H. Kocak and K.J. Palmer, *Rigorous computational shadowing of orbits of ordinary differential equations*, Numerische Mathematik **69** (1995), 401–421

Adaptive finite elements with large aspect ratio

Marco Picasso

Adaptive finite elements with large aspect ratio allow complex finite element simulations to be performed with fewer vertices. The refinement and coarsening criteria are based on anisotropic a posteriori error estimates which rely on anisotropic interpolation estimates. The goal of such estimates is to circumvent the usual regularity assumption (or equivalently the smallest angle condition), see for instance the papers of Kunert and co-workers or those of Formaggia and Perotto.

Anisotropic error estimates are nowadays available for various academic problems such advection-diffusion, Stokes, the heat equation but also for more challenging problems such as CFD or crystal growth [1, 2]. Due to recent developments in anisotropic mesh generation, three dimensional anisotropic adaptive algorithms have been implemented, showing that complex simulations can be performed on workstations.

In this workshop, I presented the error estimator and the adaptive strategy for the Laplace problem [3]. Then, I presented numerical results obtained in the framework of supersonic flows around aircrafts [4]. This is a collaboration with Dassault aviation and INRIA.

We are also working on more academic contributions, namely an anisotropic error estimator for the Crank-Nicolson scheme, and anisotropic adaptive elements for the wave equation.

References

[1] J. Narski, M. Picasso, *Adaptive finite elements with high aspect ratio for dendritic growth of a binary alloy including fluid flow induced by shrinkage*, Comp. Meth. Appl. Mech. Eng. (2007).

[2] J. Narski, M. Picasso, *Adaptive 3D finite elements with high aspect ratio for dendritic growth of a binary alloy including fluid flow induced by shrinkage*, Fluid Dyn. Mater. Proc. **4** (2007), 49–64.

[3] M. Picasso, *Adaptive finite elements with large aspect ratio based on an anisotropic error estimator involving first order derivatives*, Comp. Meth. Appl. Mech. Eng. **196** (2006), 14–23.

[4] Y. Bourgault, M. Picasso, F. Alauzet, A. Loseille, *On the use of anisotropic error estimators for computing 3D inviscid compressible flows*, submitted to Int. J. Numer. Meth. Fluids (2007).

Adaptive modeling for atomistic-to-continuum coupling methods

Serge Prudhomme

(joint work with J. Tinsley Oden, Paul T. Bauman, Leszek Demkowicz, Grant Willson, Hachmi Ben Dhia, and Nadia Elkhodja)

In this talk, we presented our preliminary work on adaptive modeling for multiscale problems involving coupling of atomistic/molecular and continuum models. The basic idea builds upon the estimation and adaptive control of modeling error as advanced in [1, 2] for general systems. These techniques were previously applied to problems of molecular statics and dynamics in [3, 5]. Extensions of the theory and methodology to complex molecular-continuum systems such as those encountered in polymer materials of interest to the nano-manufacturing industry are described here. The main ingredients involved in this approach consist of four major components:

a) A fine-scale model of a physical event is defined. Formally, one seeks a solution u to a general problem of the type

$$B(u; v) = F(v), \quad \forall v \in V \tag{1}$$

$B(\cdot,\cdot)$ being a semilinear form, V a space of test vectors, and $F(\cdot)$ a linear functional characterizing source terms or boundary data. This problem (1) is not necessarily solved or even fully available, but should be known to the extent that it can provide a datum with respect to which other models are compared.

b) Rather than the solution u to (1), it is assumed that one is interested in specific outputs of u, which mathematically consist of (linear or nonlinear) functionals Q depending on u.

c) Instead of (1), families of coarse-scale problems are constructed in the form

$$B_0(u_0; v) = F_0(v), \quad \forall v \in V \tag{2}$$

which are solvable and which should provide reasonable approximations to the solutions of the base problem (1) with respect to the quantity of interest.

d) Using theoretical estimates derived in [1, 3], one can compute estimates of the modeling error in the quantity of interest $\mathcal{E} = Q(u) - Q(u_0)$.

These steps provide the basis for adaptive control algorithms which successively upgrade the surrogate models so as to systematically reduce the modeling error $\mathcal{E}$. These algorithms are called goal-oriented adaptive methods. The key to the success of such algorithms rests on two factors: the construction of appropriate coarse-scale surrogates (typically using methods of homogenization or ensemble averaging) and the construction of appropriate interfaces between models of different scales. As an example, we showed results of a modeling error calculation for a problem of nanoindentation of an aluminum crystalline lattice interfacing a coarse-scale surrogate model obtained using a quasicontinuum approach [4]. The remarkable accuracy of the estimated error in replacing the crystalline lattice by an adaptive quasicontinuum model is shown in [5]. The quantity of interest in this case was chosen as the force supplied by the indenter.

We also described, briefly, an ongoing study of the application of these ideas to polymer materials used in semiconductor manufacturing. The base model for the polymer chains are constructed in a two-step manner: polymerization on lattices is obtained using a pseudo Monte Carlo approach and the deformation of the lattices is calculated using a molecular statics model in which the displacements of the monomers are the degrees of freedom. The continuum model is generated based on the Mooney-Rivlin theory for a hyperelastic polymer and obtained through virtual experiments of the polymer. Finally, surrogate problems are implemented using the Arlequin framework [6] that allows the coupling of the molecular model and continuum model. The objective of the adaptive approach is to predict the position and size of the interface region between the two models. Only preliminary results were shown in which estimates of the error in the Arlequin solution were calculated.

References

[1] J. T. Oden and S. Prudhomme, *Estimation of modeling error in computational mechanics*, J. Comput. Phys. **182** (2002), 496–515.

[2] M. Braack and A. Ern, *A posteriori control of modeling errors and discretization errors*, Multiscale Model. Simul **1** (2003), 221–238.
[3] J.T. Oden, S. Prudhomme, A. Romkes, and P.T. Bauman, *Multiscale modeling of physical phenomena: Adaptive control of models*, SIAM J. Scientific Computing **28** (2006), 2359–2389.
[4] E.B. Tadmor, *The Quasicontinuum Method*, Ph.D. Dissertation, Brown University (2006).
[5] S. Prudhomme, P.T. Bauman, and J.T. Oden, *Error control for molecular statics problems*, Int. J. Multiscale Comp. Eng. **4** (2006), 647-662.
[6] H. Ben Dhia and G. Rateau, *The Arlequin method as a flexible engineering design tool*, Int. J. Num. Methods. Engng. **62** (2005), 1442–1462.

Functional a posteriori estimates for mixed formulations of elliptic type boundary value problems

Sergey Repin

A posteriori error estimators are widely applied in adaptive numerical methods. In the majority of cases, they are derived by the *residual* or *dual–weighted residual* methods or with the help of *post–processing procedures* (see, e.g., [AiOd, BaSt, BaRa, BeRa, CaBa, Ra, Ve, ZiZh]). Usually, these methods attract an advanced information on properties of exact and approximate solutions in order to construct efficient error indicators.

In the report, we give a short overview of the results obtained in the framework of a different (functional) approach whose main goal is to obtain *guaranteed and computable* error bounds that do not involve mesh dependent constants and are valid for any approximation from the energy space.

Functional a posteriori error estimates are derived on purely functional grounds without attracting any specific properties of approximations or method used (such as, e.g., Galerkin orthogonality, higher regularity, superconvergence effects). They have one common form

$$\underline{M}\,(\mathcal{D}, v) \le \|u - v\|_V \le \overline{M}\,(\mathcal{D}, v) \qquad \forall v \in V, \tag{1}$$

where u is the exact solution of a problem, v is an approximation from the admissible (energy) space V, $\mathcal{D}$ denotes the set of known data of a problem and other functions and parameters which are in our disposal. The functionals $\overline{M}$ (error majorant) and $\underline{M}$ (error minorant) must be *directly computable* and such that

$$\overline{M}\,(\mathcal{D}, u) = \underline{M}\,(\mathcal{D}, u) = 0, \tag{2}$$

$$\overline{M}\,(\mathcal{D}, v_k) \to 0, \quad \underline{M}\,(\mathcal{D}, v_k) \to 0 \quad \text{as } k \to +\infty. \tag{3}$$

Two–sided functional a posteriori estimates establishes *guaranteed error bounds for conforming approximations of all the types*. If (1) is obtained for a class of boundary–value problems, then approximations computed for a problem in the class are *fully controllable*.

First a posteriori error estimates valid for any approximation in the energy space were presented in [PrSy, Mikh] (see also later publications [GaGrZa, MoMy]). However, these estimates suffer from the necessity to exactly satisfy a certain differential relation (e.g., equilibrium equation) what may lead to serious technical

difficulties. In the estimates discussed, the variables are not subject to additional differential relations and can be approximated by standard (e.g., piecewise–polynomial) functions. Originally, functional a posteriori estimates were derived for *convex variational problems* with the help of the duality methods in the calculus of variations (see [Re97a, Re97b, ReXa, ReENUMATH97, Re99]). As a simple example, we can consider the problem $\mathrm{div} A\nabla u + f = 0$ in Ω, $u = 0$ on $\partial\Omega$. The majorant of the error is given by the estimate

$$\begin{aligned} \|\nabla(u-v)\| \le & \left(\int_\Omega (A\nabla v\cdot\nabla v + A^{-1}y\cdot y - \nabla v\cdot y)dx\right)^{1/2} \\ & + C_F\left(\int_\Omega \mathrm{div} y + f)^2 dx\right)^{1/2}, \end{aligned} \tag{4}$$

where $\|z\|^2 := \int_\Omega Az\cdot z\,dx$, C_F is a constant in the Friederichs inequality, and y is an arbitrary function in $H(\Omega,\mathrm{div})$. A similar estimate holds for the Stokes problem, but in the case of non–solenoidal approximations it contains an additional term with the constant from the Babuška-Aziz-Ladyzhenskaya-Solonnikov lemma (see [LaSo]). A consequent exposition of this a posteriori error control theory can be found in [Re00] and in the book [NeRe04] .

In [Re03a], it was introduced another method based on *transformations of integral identities*. It was shown that for linear elliptic problems derived by the variational and non–variational methods approach lead to identical a posteriori estimates. New method was applied to linear parabolic problems in [Re02b, GaRe], to the Maxwell's equation in [Re07a, Re07b], to the reaction–diffusion problem in [ReSa], and to mixed formulations of elliptic problems [Re07b].

If a solution is approximated with the help of a *mixed scheme*, then in (1)–(3) u is replaced by a pair (u,p) and v by (v,q), where p is the exact solution of the dual formulation and q is its approximation (see [ReSm, ReSaSm05, Re06]).

Estimates for the *Stokes problem* were derived in [Re02a, Re04b] and for the generalized Stokes problem in [ReSt]. Estimates for flow problems in the rotating coordinate system were derived in [GoMaNeRe07] and for generalized Newtonian fluids in [BiFuRe, FuRe06, Re04b].

In [Re01], functional a posteriori estimates were applied to the estimation of the error of the 2D plane stress model with respect to a 3D model of linear elasticity. *Dimension reduction errors* for the diffusion elliptic problem has been studied in [ReSaSm04]. The errors caused by *data indeterminacy* were investigated in [Re03b].

Functional a posteriori estimates for *variational inequalities* were obtained in [BuRe, Re00a, ReVa]. Functional methods are also applicable to the analysis of *local norms* or other nonnegative quantities (see [Re04a, Re06]) and for *nonconforming approximations* (see [ReSaSm03], [LaReTo]).

In the report, a functional approach to the derivation of a posteriori error estimates for elliptic problems in mixed form was presented. Two main classes of problems considered are as follows:

- Problems whose main part is presented as $\Lambda^* A \Lambda$, where Λ is a linear bounded operator and Λ^* is its conjugate (examples are presented by diffusion, elasticity, and Maxwell problems);
- Elliptic problems whose solutions are defined in a subspace formed by the kernel of a linear bounded operator (examples are given by problems in the theory of incompressible viscous fluids).

For the dual mixed formulation we can extract them directly from the respective mixed formulation. We discuss the mathematical properties of the estimates and show that the functional majorant $\overline{M}$ is *equivalent to the error computed in a combined primal–dual norm.* In particular, for the above considered diffusion problem this combined norm is $\|\nabla(u - v)\| + \|y - p\|_{\mathrm{div}}$, where p is the exact flux and the second term is a norm in $H(\Omega, \mathrm{div})$. Similar a posteriori estimates were recently derived for the elliptic Maxwell problem [Re07a].

References

[AiOd] M. Ainsworth and J. T. Oden. *A posteriori error estimation in finite element analysis*, Wiley and Sons, New York, 2000.

[BaSt] I. Babuška and T. Strouboulis, *The finite element method and its reliability*, Oxford University Press, New York, 2001.

[BaRa] W. Bangerth and R. Rannacher, *Adaptive finite element methods for differential equations,* Birkhäuser, Berlin, 2003.

[BeRa] R. Becker and R. Rannacher, *A feed–back approach to error control in finite element methods: Basic approach and examples,* East–West J. Numer. Math., 4(1996), pp. 237-264.

[BiRe] M. Bildhauer and S. Repin, Estimates for the deviation from exact solutions of variational problems with power growth functionals, *Zapiski Nauchnych Seminarov POMI* 336(2006), 5-24.

[BiFuRe] M. Bildhauer, M. Fuchs and S. Repin, *A posteriori error estimates for stationary slow flows of power–law fluids,* Journal of Non-Newtonian Fluid Mechanics (in press).

[BuRe] H. Buss and S. Repin. A posteriori error estimates for boundary–value problems with obstacles. In *Proceedings of 3nd European Conference on Numerical Mathematics and Advanced Applications, Jyuvaskyla, 1999*,162–170, World Scientific, 2000.

[CaBa] C. Carstensen and S. Bartels. Each averaging technique yields reliable a posteriori error control in FEM on unstructured grids. I: Low order conforming, nonconforming, and mixed FEM, Math. Comp., 71(2002), pp. 239, 945-969.

[FuRe06] M. Fuchs and S. Repin. Estimates for the deviation from the exact solutions of variational problems modeling certain classes of generalized Newtonian fluids, *Math. Meth. Appl. Sci.*, 29 (2006), pp. 2225–2244.

[GaGrZa] H. Gaevskii, H., K. Gröger, and K. Zacharias, *Nichtlineare Operator-gliechungen and Operatordifferentialgleiichungen,* Akademie-Verlag, Berlin, 1974.

[GaRe] A. Gaevskaya and S. Repin. A posteriori error estimates for approximate solutions of linear parabolic problems, *Differential Equations*, 41 (2005), 7, pp. 970–983.

[GoNeRe] E. Gorshkova, P. Neittaanmaki, and S. Repin. Comparative study of a posteriori error estimates for the Stokes problem, Proc. of 6th European Conference on Numerical Mathematics and Advanced Applications, Springer, Berlin, 2006, 255-262,

[GoMaNeRe07] E. Gorshkova, A. Mahalov, P. Neittaanmaki, and S. Repin. A posteriori error estimates for viscous flow problems with rotation, *J. Math. Sci. (New York)*, 142(2007), 1, 1749–1762.

[LaSo] O. A. Ladyzenskaja and V. A. Solonnikov, Some problems of vector analysis, and generalized formulations of boundary value problems for the Navier-Stokes equation, *Zap. Nauchn, Sem. Leningrad. Otdel. Mat. Inst. Steklov. (LOMI)*, 59(1976), pp. 81–116 (in Russian).

[LaReTo] R. Lazarov, S. Repin, and S. Tomar, *Functional a posteriori error estimates for Discontinuous Galerkin method,* Radon Institute of Computational and Applied Mathematics, Preprint 2006-40, Linz.

[Mikh] S. G. Mikhlin, *Variational methods in mathematical physics*, Pergamon, Oxford, 1964.

[MoMy] P.Mosolov and V.Myasnikov, *Mechanics of rigid plastic bodies*, Nauka, Moscow, 1981 (in Russian).

[NeRe04] P. Neittaanmäki and S. Repin. *Reliable methods for computer simulation. Error control and a posteriori estimates*, Elsevier, New York, London, 2004.

[NeRe01] P. Neittaanmäki and S. Repin. A posteriori error estimates for boundary–value problems related to the biharmonic operator, *East-West J.Numer. Math.*, 9 (2001), 2, 157-178.

[PrSy] W. Prager and J. L. Synge, *Approximation in elasticity based on the concept of function space,* Quart. Appl. Math. 5(1947), pp. 241-269.

[Ra] R. Rannacher. The dual-weighted-residual method for error control and mesh adaptation in finite element methods. In *The mathematics of finite elements and applications X, MAFELAP 1999. Proceedings of the 10th conference, Brunel Univ., Uxbridge, Middlesex, GB, June 22-25, 1999 (ed. J. Whiteman).* Elsevier, Amsterdam, 2000, pp 97-116.

[Re97a] S. Repin. A posteriori error estimation for problems with power growth functional, *Zapiski Nauchn. Semin. POMI*, 249 (1997), 244–255.

[Re97b] S. Repin. A posteriori error estimation for nonlinear variational problems by duality theory, *Zapiski Nauchnych Seminarov POMI*, 243(1997) 201–214.

[ReENUMATH97] S. Repin. A posteriori error estimation for approximate solutions of variational problems by duality theory. In *Proceedings of 2nd European Conference on Numerical Mathematics and Advanced Applications,Heidelberg, 1997*, 524–531, World Scientific, 1999.

[Re96] S. Repin. Errors of finite element method for perfectly elasto-plastic problems, *Math. Models. Meth. Appl. Sci. (M^3AS)*, 6 (1996), 587–604.

[Re99] S. Repin. A unified approach to a posteriori error estimation based on duality error majorants. *Mathematics and Computers in Simulation* 50 (1999), 313–329.

[Re00] S. Repin. A posteriori error estimation for variational problems with uniformly convex functionals, *Mathematics of Computations*, 69 (2000), 230, 481–500.

[Re00a] S. Repin. Estimates of deviations from exact solutions of elliptic variational inequalities. *Zapiski Nauchn. Semin. V.A. Steklov Mathematical Institute in St.-Petersburg (POMI)*, 271 (2000), 188–203.

[Re01] S. Repin. Estimates for errors in two-dimensional models of elasticity theory, *J. Math. Sci. (New York)*, 106 (2001), 3, 3027–3041.

[Re02a] S. Repin. A posteriori estimates for the Stokes problem, *Journal of Math. Sciences* 109 (2002), 5, 1950–1964.

[Re02b] Estimates of deviation from exact solutions of initial-boundary value problems for the heat equation, *Rend. Mat. Acc. Lincei*, 13(2002), pp. 121-133.

[Re03a] S. Repin. Two-Sided estimates of deviation from exact solutions of uniformly elliptic equations, *Amer. Math. Soc. Transl. Series 2*, 209 (2003), 143–171.

[Re03b] S. Repin. A posteriori error estimates with account of indeterminacy of the problem data. *Russ. J. Numer. Anal. Math. Modelling*, 18 (2003), n. 6, 507-519.

[Re04a] S. Repin. A posteriori estimates in local norms. *J. Math. Sci. (N. Y.)* 124 (2004), no. 3, 5026–5035.

[Re04b] S. Repin. Functional type a posteriori error estimates for approximate solutions of problems with incompressibility condition. In *European Congress on Computational Methods in Applied Sciences and Engineering, ECCOMAS 2004, P.Neittaanmäki, T. Rossi, K. Majava and O. Pironeau (eds.), O. Nevanlinna and R. Rannacher (assoc. eds.), Jyväskylä, 24-28 July, 2004* (electronic).

[Re06] S. Repin. Functional Approach to Locally Based A Posteriori Error Estimates for Elliptic and Parabolic Problems, *Proc. 6th European Conference on Numerical Mathematics and Advanced Applications*, Springer, Berlin, 2006, 133-148.

[Re07a] S. Repin. Functional a posteriori estimates for the Maxwell's problem, *J. Math. Sci. New York*, 142(2007), 1, 1821–1827.

[Re07b] S. Repin. On the derivation of functional a posteriori estimates from integral identities, in *Advances in Numerical Mathematics; Proc. Int. Conf. 60th jubilee Yu. Kuznetsov; eds. W. Fitzgibbon, R. Hoppe, J. Peiaux, O. Pironneau, Yu. Vassilevski*, Moscow 2006, 217–242.

[ReSa] S. Repin and S. Sauter, Functional A Posteriori Estimates for the Reaction-Diffusion Problem, *C. R. Acad. Sci. Paris, Ser. 1*, 343(2006), 349–354.

[ReSm] S. Repin and A. Smolianski, *Functional-type a posteriori error estimates for mixed finite element methods, Russian J. Numer. Anal. Math. Modelling* 20 (2005), 4, pp. 365–382.

[ReSaSm03] S. Repin, S. Sauter, and A. Smolianski. A posteriori error estimation for the Dirichlet problem with account of the error in approximation of boundary conditions. *Computing*, (2003), 3, 147-168.

[ReSaSm04] S. Repin, S. Sauter, and A. Smolianski. A posteriori estimation of dimension reduction errors for elliptic problems in thin domains. *SIAM J. Numer. Anal.*, 42 (2004), 4, 1435–1451.

[ReSaSm05] S. Repin, S. Sauter, and A. Smolianski. *Two-Sided A Posteriori Error Estimates for Mixed Formulations of Elliptic Problems,* Preprint 21-2005, Institute of Mathematics, University of Zurich, to appear in SIAM J. Numer. Anal.

[ReSt] S. Repin and R. Stenberg. A posteriori error estimates for the generalized Stokes problem, *J. Math. Sci. (New York)*, 142(2007), 1, 1828–1843.

[ReVa] S. Repin and J. Valdman, *A posteriori error estimates for problems with nonlinear boundary conditions,* Radon Institute of Computational and Applied Mathematics, Preprint 2006-25, Linz.

[ReXa] S. Repin and L. Xanthis. A posteriori error estimation for elasto-plastic problems based on duality theory, *Comput. Methods Appl. Mech. Engrg.*, 138 (1996), 317-339.

[Ve] R. Verfürth, *A review of a posteriori error estimation and adaptive mesh-refinement techniques* Wiley and Sons, Teubner, New-York, 1996.

[ZiZh] O. C. Zienkiewicz and J. Z. Zhu, *A simple error estimator and adaptive procedure for practical engineering analysis,* Internat. J. Numer. Meth. Engrg. 24(1987) pp. 337-357.

Optimal cardinality of an adaptive finite element method

Kunibert G. Siebert

(joint work with J. Manuel Cascon, Christian Kreuzer, and Ricardo H. Nochetto)

We report on the recent work [2] where we analyze convergence and optimal cardinality of the standard adaptive finite element method (AFEM)

$$\mathsf{SOLVE} \to \mathsf{ESTIMATE} \to \mathsf{MARK} \to \mathsf{REFINE}$$

for solving adaptive approximations to the weak solution of the symmetric, elliptic problem

$$-\operatorname{div}(\mathbf{A}\nabla u) + c\,u = f \quad \text{in } \Omega, \qquad u = 0 \quad \text{on } \partial\Omega. \tag{1}$$

Hereafter, Ω is a bounded, polyhedral domain in $\mathbb{R}^d$, $d \geq 2$, that is triangulated by some conforming triangulation $\mathcal{T}_0$, $\mathbf{A}\colon \Omega \mapsto \mathbb{R}^{d\times d}$ is piecewise Lipschitz over $\mathcal{T}_0$ and uniformly symmetric positive definite, $c \in L^\infty(\Omega)$ is nonnegative, and $f \in L^2(\Omega)$. We denote given data of (1) by $\mathbf{D} = (\mathbf{A}, c, f)$.

Even though adaptivity has been a fundamental tool of engineering and scientific computing for about three decades, the convergence analysis is rather recent. It started with Dörfler [5], who introduced a crucial marking, from now on called

Dörlfer marking, and proved strict energy error reduction for the Laplacian provided the initial mesh $\mathcal{T}_0$ satisfies a fineness assumption. Morin, Nochetto, and Siebert [7, 8] showed that such strict energy error reduction cannot be expected in general. Introducing the concept of data oscillation, the interior node property, and separate Dörlfer marking for estimator *and* oscillation, they proved convergence of AFEM without restrictions on $\mathcal{T}_0$. The latter result, however, is only valid for $\mathbf{A}$ being piecewise constant on $\mathcal{T}_0$ and vanishing c. Inspired by the work by Chen and Feng [3], Mekchay and Nochetto [6] extended this result to general second order elliptic operators upon dealing with the new concept of *total error*, namely the sum of energy error plus oscillation. They proved that AFEM is a contraction for the total error, a property that will turn out to be here essential as well. Recently, Diening and Kreuzer [4] proved a similar property for the p-Laplacian but avoiding marking for oscillation.

Quasi-optimal convergence rates for AFEM, expressing energy error decay in terms of number of degrees of freedom (DOFs) as dictated by nonlinear approximation theory, were first proved by Binev, Dahmen and DeVore [1]. They resorted to a crucial, but somewhat artificial coarsening step. Coarsening was later removed by Stevenson [11], who developed an optimality theory for a much more realistic AFEM but still including an inner loop to deal with oscillation. Both papers are restricted to the Laplace operator and rely on the the interior node property and a suitable marking for oscillation.

When marking with respect to two quantities such as estimator and oscillation in the algorithm by Morin, Nochetto, and Siebert, the role of marking becomes critical for proving optimality. The comparison of separate and collective marking for two quantities in a simplified scenario reveals that an appropriate choice of marking parameters becomes critical. Indeed, separate marking might be suboptimal and should thus be avoided, whereas collective marking leads to optimal convergence rates. This insight explains why Binev, Dahmen, and DeVore[1] use a coarsening step to recover optimal cardinality, and Stevenson [11] separates marking for estimator and oscillation by the additional inner loop.

Relying on the exact Ritz-Galerkin solutions U_k to (1) in a sequence of conforming and nested finite element spaces $\mathbb{V}_k \subset H^1_0(\Omega)$ over triangulations $\mathcal{T}_k$, the standard residual estimator $\mathcal{E}_k(U_k, \mathbf{D})$, minimal Dörfler marking solely for the estimator, and minimal refinement by bisection of marked elements, we show that AFEM is a contraction for the sum of energy error and scaled estimator, namely

$$|||u - U_{k+1}|||^2_\Omega + \gamma^2 \mathcal{E}^2_{k+1}(U_{k+1}, \mathbf{D}) \leq \alpha^2 \Big(|||u - U_k|||^2_\Omega + \gamma^2 \mathcal{E}^2_k(U_k, \mathbf{D}) \Big) \tag{2}$$

with suitable constants $\alpha \in (0, 1)$ and $\gamma > 0$. Even though the energy error is monotone, strict error reduction fails when $U_{k+1} = U_k$ and thus $|||u - U_k|||_\Omega = |||u - U_{k+1}|||_\Omega$, compare with [7, 8] for details. Although the residual estimator is not monotone in general, in this situation it exhibits a strict reduction, this is $\mathcal{E}_{k+1}(U_k, \mathbf{D}) \leq \delta \mathcal{E}_k(U_k, \mathbf{D})$ with $\delta \in (0, 1)$. The contraction property (2) is then a consequence of the scenario described above or a strict reduction of the energy error in combination with local Lipschitz-continuity of the estimator.

Realizing that contraction of AFEM solely relies on the *upper bound*, we utilize the *continuous lower bound* to see

$$|||u - U_k|||_\Omega^2 + \mathcal{E}_k^2(U_k, \mathbf{D}) \approx |||u - U_k|||_\Omega^2 + \mathrm{osc}_k^2(U_k, \mathbf{D}).$$

Hence, the sum of energy error plus oscillation, the so-called *total error*, is equivalent to the quantity being strictly reduced by AFEM and it satisfies a Cea's Lemma. This motivates the definition of the approximation class $\mathbb{A}_s$ which states that $(u, \mathbf{D})$ belongs to $\mathbb{A}_s$, if the total error can be approximated within any tolerance $\epsilon > 0$ with $O(\epsilon^{-s})$ degrees of freedom. Even for a linear PDE with variable coefficients like (1), oscillation and solution couple in a nonlinear fashion. As an outcome, an important pending issue is a complete characterization of $\mathbb{A}_s$.

Assuming certain restrictions on the initial triangulation [12] and that the marking parameter of Dörfler marking is sufficiently small, we finally show that AFEM achieves for $(u, \mathbf{D}) \in \mathbb{A}_s$ the asymptotic decay rate s in terms of degrees of freedom as described by the membership in $\mathbb{A}_s$, this is

$$\big(|||u - U_k|||_\Omega^2 + \mathrm{osc}_k^2(U_k, \mathbf{D})\big)^{1/2} \leq C\big(\#\mathcal{T}_k - \#\mathcal{T}_0\big)^{-s}. \tag{3}$$

In contrast to former optimality proofs [1, 11], the presented analysis stays within the class of conforming meshes, which is necessary when dealing with oscillation in the jump residual. Using the ideas of Stevenson [11], in the proof of (3) we combine the contraction property of AFEM, a quasi-monotonicity property of oscillation, a localized upper bound with an optimal complexity of refinement by bisection [1, 11].

In the talk we have analyzed a standard AFEM as it is used in practice and provide a theory for convergence and optimality. The first convergence result for such a standard AFEM is due to Morin, Siebert, and Veeser [10]. They recently proved for a larger problem class and more general marking strategies plain convergence of AFEM but without an error reduction property. Relying on Dörfler marking we are able to prove a stronger result for selfadjoint elliptic operators of the form (1), namely contraction of the quasi-error and quasi-optimal cardinality.

In all other convergence and optimality results, the standard form of AFEM is first altered and then the modified algorithms are analyzed. Because of theoretical needs additional ingredients, such as the interior node property and marking for oscillation [6, 7, 8, 9], a coarsening step [1], or an additional inner loop to decrease oscillation relative to the estimator [11], are added to AFEM. We would like to stress that removing these ingredients is very important from a practical point of view. The interior node property enforces six bisections of marked elements in three space dimensions and thus increases the number of DOFs between two iterations drastically. In fact, computational resources can be used more efficiently with fewer element refinements. Last but not least, in contrast to modified versions of AFEM, the standard form only needs *one single* parameter, namely the parameter of Dörfler marking. Hence, it is not necessary to fit several parameters, which in turn makes the resulting algorithm more robust.

References

[1] P. Binev, W. Dahmen, and R. DeVore, *Adaptive finite element methods with convergence rate*, Numer. Math. 97 (2004), 219-268.

[2] J. Manuel Cascon, Christian Kreuzer, Ricardo H. Nochetto, and Kunibert G. Siebert *Quasi-Optimal Convergence Rate for an Adaptive Finite Element Method*, Preprint 009/2007, Institut für Mathematik, Universität Augsburg.

[3] Z. Chen, J. Feng, *An adaptive finite element algorithm with reliable and efficient error control for linear parabolic problems*, Math. Comp. 73 (2004), 1167–1193.

[4] L. Diening and C. Kreuzer, *Linear Convergence of an adaptive finite element method for the p-Laplacian equation*, Preprint No. 03/2007, Institut für Mathematik, Universität Freiburg, to appear in SINUM.

[5] W. Dörfler, *A convergent adaptive algorithm for Poisson's equation*, SIAM J. Numer. Anal. 33 (1996), 1106-1124.

[6] K. Mekchay and R.H. Nochetto, *Convergence of adaptive finite element methods for general second order linear elliptic PDEs*, SIAM J. Numer. Anal. 43, (2005), 1043–1068.

[7] P. Morin, R. H. Nochetto, and K. G. Siebert, *Data oscillation and convergence of adaptive FEM*, SIAM J. Numer. Anal. 38 (2000), 466–488.

[8] P. Morin, R. H. Nochetto, and K. G. Siebert, *Convergence of adaptive finite element methods*, SIAM Rev. 44, (2002), 631–658.

[9] P. Morin, R. H. Nochetto, and K. G. Siebert, *Local problems on stars: a posteriori error estimation, convergence, and performance*, Math. Comp. 72 (2003), 1067–1097.

[10] P. Morin, K.G. Siebert, A. Veeser, *A basic convergence result for conforming adaptive finite elements*, Preprint 007/2007, Institut für Mathematik, Universität Augsburg.

[11] R. Stevenson, *Optimality of a standard adaptive finite element method*, Found. Comput. Math. Online. DOI 10.1007/s10208-005-0183-0, (2006).

[12] R. Stevenson, *The completion of locally refined simplicial partitions created by bisection*, Preprint No. 1336, 13 pages, Department of Mathematics, Utrecht University, September 2005. Corrected version, October 2006.

Optimal adaptive finite element and wavelet methods

Rob Stevenson

(joint work with Christoph Schwab)

In this talk, we discuss optimal convergence of adaptive finite element and adaptive wavelet methods for solving operator equations.

Adaptive *finite element* methods for solving elliptic boundary value problems have the potential to produce a sequence of approximations to the solution that converges with a rate that is optimal in view of the polynomial order that is applied, also in the, common, situation that finite element approximations with respect to uniformly refined partitions exhibit a reduced rate due to a lacking (Sobolev) regularity of the solution. The basic idea of an adaptive finite element method is, given some finite element approximation, to create a refined partition by subdividing those elements where local error estimators indicate that the error is large, and then, on this refined partition, to compute the next approximation, after which the process can be repeated. Although, because of their success in practice, during the last 30 years the use of these adaptive methods became more and more widely spread, apart from results in the one-dimensional case by Babuška

and Vogelius ([1]), their convergence was not shown before the work by Dörfler ([9]), that was later extended by Morin, Nochetto and Siebert ([11]).

Although these results meant a break through in the theoretical understanding of adaptive methods, they do not tell anything about the rate of convergence, and so, in particular, they do not show that adaptive methods are more effective than, or even competitive with non-adaptive ones in the situation that the solution has a lacking regularity.

In [2], Binev, Dahmen and DeVore developed an adaptive finite element method which they showed to be of optimal computational complexity. Whenever for some $s > 0$, the solution is in the approximation class $\mathcal{A}^s$, meaning that there exists a sequence of partitions of the domain into n elements such that the best finite element approximation with respect to this partition has an error in energy norm of order n^{-s}, then the adaptive method produces a sequence of approximations that converge with the same rate, where, moreover, the cost of computing such an approximation is of the order of the number of elements in the underlying partition. A combination of the (near) characterization of $\mathcal{A}^s$ in terms of Besov spaces from [3], and Besov regularity theorems from [7, 6], indicate that under very mild conditions the value of s is indeed only restricted by the polynomial order.

The key to obtain the optimal computational complexity result was the addition of a so-called coarsening or derefinement routine to the method from [11], that has to be applied after each fixed number of iterations, as well as, in view of the cost, to replace the exact Galerkin solvers by inexact ones.

In this talk, we show that the addition of coarsening can be avoided. We present an adaptive finite element method, that, except that we solve the Galerkin systems inexactly, is very similar to the one from [11], and show that it has optimal computational complexity. In doing so, we restrict ourselves to the model case of the Poisson equation in two space dimensions, linear finite elements, and partitions that are created by newest vertex bisection ([15]). Our results, however, generalize to any space dimension ([14]), finite elements of any order, and to differential operators $\nabla \cdot A\nabla$ with A symmetric positive definite, and piecewise constant with respect to the initial partition.

Adaptive *wavelet* method for solving well posed operator equations were introduced by Cohen, Dahmen and DeVore in [4, 5]. So far the most promising numerical results were obtained with the method from [4]. In this talk, we present some modifications of this method that result in quantitative improvements. Most importantly, as with adaptive finite element methods we show that coarsening can be avoided ([10]).

In the last part of this talk, we discuss the application of the adaptive wavelet method for solving PDEs in high space dimensions. When solving elliptic PDEs of say second order in n space dimensions, using (adaptive) wavelet or finite element methods of order d, the best possible rate in energy norm is $\mathcal{O}(N^{-d/n})$, with N being the number of degrees of freedom. When applying hyperbolic cross approximation (sparse grids), the curse of dimensionality can be avoided in the sense that

a rate $\mathcal{O}(N^{-d})$ can be realized. This, however, requires L_2 boundedness of certain mixed derivatives of the solution, which is satisfied actually in exceptional cases only. In [12], it was shown that best N-term approximations in tensor product wavelet bases realize this rate $\mathcal{O}(N^{-d})$ under very mild regularity conditions.

The rate of best N-term approximation can be realized computationally with adaptive wavelet methods, *assuming* that the operator in wavelet coordinates, i.e., the (infinite) stiffness matrix is sufficiently close to a computable sparse matrix. Due to the higher rates of N-term approximations, for tensor product wavelets the requirements concerning near-sparsity are much stronger. Nevertheless, we were able to show that these requirements are satisfied for general partial differential operators with sufficiently smooth coefficients (cf. [13]).

A point of concern is the behaviour of the "hidden constant" in front of the rate. Without taking special care, one easily ends up with a constant that grows exponentially with n, making the method unpractical except for small n. Restricting ourselves to operators with constant coefficients, we present an adaptive wavelet method that produces approximations of length N that up to some absolute constant are as good as best N-term approximations, at the cost of CnN operations, with C being another absolute constant ([8]).

References

[1] I. Babuška, and M. Vogelius. Feedback and adaptive finite element solution of one-dimensional boundary value problems. *Numer. Math.*, 44(1), 1984.

[2] P. Binev, W. Dahmen, and R. DeVore. Adaptive finite element methods with convergence rates. *Numer. Math.*, 97(2):219 – 268, 2004.

[3] P. Binev, W. Dahmen, R. DeVore, and P. Petruchev. Approximation classes for adaptive methods. *Serdica Math. J.*, 28:391–416, 2002.

[4] A. Cohen, W. Dahmen, and R. DeVore. Adaptive wavelet methods for elliptic operator equations – Convergence rates. *Math. Comp*, 70:27–75, 2001.

[5] A. Cohen, W. Dahmen, and R. DeVore. Adaptive wavelet methods II - Beyond the elliptic case. *Found. Comput. Math.*, 2(3):203–245, 2002.

[6] S. Dahlke. Besov regularity for elliptic boundary value problems in polygonal domains. *Appl. Math. Lett.*, 12(6):31–36, 1999.

[7] S. Dahlke and R. DeVore. Besov regularity for elliptic boundary value problems. *Comm. Partial Differential Equations*, 22(1 & 2):1–16, 1997.

[8] T J. Dijkema, Ch. Schwab, and R.P. Stevenson. An adaptive wavelet method for solving high-dimensional elliptic PDEs. Technical report, 2007. In preparation.

[9] W. Dörfler. A convergent adaptive algorithm for Poisson's equation. *SIAM J. Numer. Anal.*, 33:1106–1124, 1996.

[10] T. Gantumur, H. Harbrecht, and R.P. Stevenson. An optimal adaptive wavelet method without coarsening of the iterands. *Math. Comp.*, 77:615–629, 2007.

[11] P. Morin, R. Nochetto, and K. Siebert. Data oscillation and convergence of adaptive FEM. *SIAM J. Numer. Anal.*, 38(2):466–488, 2000.

[12] P.-A. Nitsche. Best N-term approximation spaces for tensor product wavelet bases. *Constr. Approx.*, 41(1):49–70, 2006.

[13] Ch. Schwab and R.P. Stevenson. Adaptive wavelet algorithms for elliptic PDEs on product domains. *Math. Comp.*, 2007. To appear.

[14] R.P. Stevenson. The completion of locally refined simplicial partitions created by bisection. Technical report, Department of Mathematics, Utrecht University, October 2006. To appear in *Math. Comp.*

[15] R.P. Stevenson. Optimality of a standard adaptive finite element method. *Found. Comput. Math.*, 7(2):245–269, 2007.

Optimal control to determine a continuum phase change model from molecular dynamics

Anders Szepessy
(joint work with Erik von Schwerin)

The dynamics of dendritic growth of a crystal in an undercooled melt is determined by macroscopic diffusion-convection of heat and capillary forces acting on length scales compared to the nanometer width of the solid-liquid interface. Its modeling is useful for instance in processing techniques based on casting.

The phase field method is widely used to study evolution of such microstructures of phase transformations on a continuum level; it couples the energy equation to a phenomenological Allen-Cahn/Ginzburg-Landau equation modeling the dynamics of an order parameter determining the solid and liquid phases, including also stochastic fluctuations to obtain the qualitative correct result of dendritic side branching and nucleation. This lecture presented ideas and computational results to derive stochastic phase field models from atomistic formulations by coarse-graining molecular dynamics.

The phase field model for modeling a liquid solid phase transformation is an Allen-Cahn/Ginzburg-Landau equation coupled to the energy equation

$$\begin{aligned} \partial_t \phi &= \operatorname{div}(k_1 \nabla \phi) - k_0\big(f'(\phi) + g'(\phi) k_4 T\big) + \text{noise} \\ \partial_t\big(c_v T + k_2 g(\phi)\big) &= \operatorname{div}(k_3 \nabla T) \end{aligned} \tag{1}$$

with a double well potential f having local minima at ± 1, smoothed step function g, temperature T and specific heat c_v. The phase field variable $\phi : \mathbb{R}^d \times [0,\infty) \to [-1,1]$ interprets the solid and liquid phases as the domains $\{x \in \mathbb{R}^d : \phi(x) > 0\}$ and $\{x \in \mathbb{R}^d : \phi(x) < 0\}$ respectively. To have such an implicit definition of the phases, as in the level set method, is a computational advantage compared to a sharp interface model, where the necessary direct tracking of the interface introduce computational drawbacks. This phenomenological phase-field model, with free energy potentials motived by thermodynamics, has therefore become a popular and effective computational method to solve problems with complicated microstructures of dendrite and eutectic growth. The phase-field model has mathematical wellposedness and convergence to sharp interface results.

Assuming that the reaction term in the Allen-Cahn equation takes a given form, e.g. a standard choice is

$$\begin{aligned} f(\phi) &:= (1-\phi^2)^2 \\ g(\phi) &:= \frac{15}{16}\Big(\frac{1}{5}\phi^5 - \frac{2}{3}\phi^3 + \phi\Big) + \frac{1}{2}, \end{aligned}$$

then the parameters k_0, k_1, k_2, k_3, k_4 in the phase-field model has been determined from atomistic molecular simulations [1]. The evolution of the phase interface

depends on the orientation of the solid crystal; this is modeled by an anisotropic matrix k_1. Added noise to system (1) is also important, e.g. to obtain sidebranching dendrites [2].

Phase changes can be modeled on an atomistic level by molecular dynamics or kinetic Monte Carlo methods. This lecture presented results combining computations and analysis to derive a stochastic phase field model by directly coarse-graining molecular dynamics, in an adaptive model approach, to determine also the reaction term (i.e. f and g) and the noise. This is made in three steps presented in [3] and [4]:

- to give a precise quantitative atomistic definition of the phase-field variable based on the local potential energy,
- to introduce an atomistic molecular dynamics model based on Smoluchowski dynamics, and
- to derive and compute the dynamics for the coarse-grained phase-field based on optimal control approximation of the atomistic model.

References

[1] J.J Hoyt, M. Asta, A. Karma, *Atomistic and continuum modeling of dendritic solidification*, Materials Science Engineering R-Reports **4**1 (2003), 121–163.
[2] A. Karma, W.J. Rappel, *Phase-field model of dendritic side branching with thermal noise*, Phys Rev. E. **6**0 (1999), 3614–3625.
[3] A. Szepessy, *Atomistic and continuum models for phase change dynamics*, proceedings of International Congress for Mathematicians, Madrid 2006.
[4] E. von Schwerin, *A stochastic phase-field model computed from coarse-grained molecular dynamics*, thesis draft, `www.nada.kth.se/∼schwerin`

A posteriori error estimation and adaptivity for PDE-constrained optimization

Boris Vexler

(joint work with Dominik Meidner, Winnifried Wollner, and Olaf Benedix)

We present a general approach for error estimation and adaptivity for optimization problems governed by partial differential equations. We treat this topic for a large class of optimization problems involving optimal control and parameter identification problems governed by either elliptic or parabolic partial differential equations.

An abstract optimization problem is given by minimization of a cost functional $J(q, u)$ which depends on the state variable $u \in V$ and the control (parameter) variable $q \in Q$, with Hilbert spaces V and Q. These variables are coupled through the state equation

$$A(q, u) = f,$$

where A denotes a (nonlinear) differential operator and f represents the given data. The optimization problem is then formulated as follows:

$$\begin{cases} \text{Minimize } J(q,u), \quad u \in V,\, q \in Q_{\text{ad}}, \\ A(q,u) = f, \end{cases}$$

where $Q_{\text{ad}} \subset Q$ denotes the set of admissible controls, which is usually given through some box constraints.

For numerical treatment this infinite dimensional optimization problem has to be discretized using a suitable discretization scheme for the state equation and a discrete subspace for the control variable. Let (q_σ, u_σ) be a solution of the discretized optimization problem. Our aim is to derive a posteriori error estimates for the error between the solutions to the continuous and the discrete problem. A crucial point for our error analysis is the choice of a quantity, which describes the goal of the computation. If this quantity coincides with the cost functional, we have to estimate the error

$$J(q,u) - J(q_\sigma, u_\sigma).$$

In a more general case, we suppose $I\colon Q \times V \to \mathbb{R}$ to be a given functional describing the quantity of interest. Then, the error to be estimated is

$$I(q,u) - I(q_\sigma, u_\sigma).$$

The consideration of quantities of interest is important, for instance, in the context of parameter identification and model calibration problems.

In the first part of this talk we present a posteriori error estimators for optimization problems governed by parabolic equations. This is an extension of the work in [1, 2, 3, 4], where stationary optimization problems were considered. The state equation is discretized by discontinuous finite elements in time and usual conforming finite elements in space. In order to set up an efficient adaptive algorithm we separate the influences of the time and space discretizations on the error in the quantity of interest. This allows to balance different types of errors and successively to improve the accuracy by construction of locally refined meshes for time and space discretizations, see [5]. Moreover, this concept enables separate refinement of the spatial meshes in different times steps (so called dynamic meshes), which is important for numerical treatment of problems with complex dynamical behavior, see [6].

In the second part of the talk we discuss a posteriori error estimation for optimization problems involving inequality constraints. The presence of pointwise inequality constraints on the control variable leads to an optimality condition which is either a variational inequality or involves an additional Lagrange multiplier. Another difficulty in deriving error estimates is the fact that the control variable is not expected to be sufficiently smooth (due to inequality constrains), and therefore the approximation of (interpolation) weights involved in the error estimator can not be treated in a usual way. To cope with this problem we employ a post-processing step for the control variable based on the optimality condition formulated via a projection formula. This allows us to derive error estimates for

the error with respect to the cost functional as well as for the error with respect to a given quantity of interest, see [7]. For the error estimation with respect to a quantity of interest an additional (dual) linear-quadratic optimal control problem is utilized describing the sensitivity with respect to this quantity.

In the last part of the talk we discuss our recent results on a posteriori error estimation for optimal control problems with inequality constraints on the state variable. The presence of such *state constraints* introduces strong singularities at the boundary between active and inactive sets. The Lagrange multipliers associated to the state constraints are usually regular Borel measures, i.e. in the dual space of the space of continuous functions $C(\bar{\Omega})$. We derive an error representation formula which contains usual terms involving residuals and weights for the state and the adjoint variable as well as an additional term involving the duality product of the Lagrange multiplier and the discretization error in the state variable. For the last term we suggest an approximation exploiting the adjoint equation.

Different numerical examples illustrate the behavior of our method.

References

[1] R. Becker, H. Kapp, and R. Rannacher, *Adaptive finite element methods for optimal control of partial differential equations: Basic concept,* SIAM J. Cont. Opt. **39(1)** (2000), 113-132.

[2] R. Becker and R. Rannacher, *An optimal control approach to a posteriori error estimation in finite element methods,* In Acta Numerica 2001 (A. Iserles, ed.), Cambridge University Press, Cambridge (2001), 1–102.

[3] R. Becker and B. Vexler, *A posteriori error estimation for finite element discretization of parameter identification problems,* Numer. Math. **96(3)** (2004), 435-459.

[4] R. Becker and B. Vexler, *Mesh refinement and numerical sensitivity analysis for parameter calibration of partial differential equations,* J. Comp. Phys. **206(1)** (2005), 95-110.

[5] D. Meidner and B. Vexler, *Adaptive space-time finite element methods for parabolic optimization problems*, SIAM J. Control Optim. **46(1)** (2007), 116–142.

[6] M. Schmich and B. Vexler, *Adaptivity with Dynamic Meshes for Space-Time Finite Element Discretizations of Parabolic Equations*, SIAM J. Sci. Comput. (2007), to appear.

[7] B. Vexler and W. Wollner, *Adaptive finite elements for elliptic optimization problems with control constraints*, SIAM J. Control Optim. (2007), submitted.

Adaptive finite element methods for optimal control problems with control constraints

Winnifried Wollner

(joint work with Boris Vexler)

The talk is about posteriori error estimation for optimization problems subject to an elliptic partial differential equation and pointwise inequality constraints on the control variable, so called box constraints. For a posteriori error estimates with respect to natural norms we refer to [1, 6, 7, 8, 9]. Here we show how to extend the ideas of the DWR-method to estimate the error in an arbitrary functional introduced in [2, 3, 4], details may be found in [12]. A similar approach can be found in [5] where only the error in the cost functional is considered.

To introduce notation we consider the following model optimization problem:

$$\min_{Q^{\mathrm{ad}}\times V} J(q,u) = \frac{1}{2}\|u-u^d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|q\|^2_{L^2(\Omega)} \tag{1a}$$

$$\text{s.t. } a(q,u)(\phi) = f(\phi) \quad \forall\, \phi \in V \tag{1b}$$

with $\alpha > 0$, $u^d \in L^2(\Omega)$, $V = H^1_0(\Omega)$ and

$$a(q,u)(\phi) = f(\phi) \quad \forall\, \phi \in V$$

being the weak formulation of an elliptic PDE, here we consider

$$\begin{aligned} -\Delta u + u^3 + u &= f + q \quad \text{on } \Omega, \\ u &= 0 \quad \text{on } \partial\Omega, \end{aligned}$$

and the admissible set is given as

$$Q^{\mathrm{ad}} = \{q \in L^2(\Omega) \,|\, a \le q(x) \le b \text{ a.e.}\}$$

with $a, b \in \mathbb{R}$, $a < b$. However more general problems can be considered, for instance other types of cost functionals are possible, for details see [12].

We introduce the Lagrangian associated with the PDE, and inequality constraints:

$$\mathcal{L}(q,u,z,\mu^-,\mu^+) = J(q,u) + f(z) - a(q,u)(z) + (\mu^-, q-a)_{L^2(\Omega)} + (\mu^+, b-q)_{L^2(\Omega)}.$$

Than we can derive by standard arguments, cf. [11] that a solution (q,u) of (1) fulfills the following KKT-system:
There exists $z \in V$, μ^-, $\mu^+ \in L^2(\Omega)$ such that:

$$\mathcal{L}'_q(q,u,z,\mu^-,\mu^+) = 0 \quad \forall\, \partial q \in L^2(\Omega), \tag{2a}$$

$$\mathcal{L}'_u(q,u,z,\mu^-,\mu^+) = 0 \quad \forall\, \partial u \in V, \tag{2b}$$

$$\mathcal{L}'_z(q,u,z,\mu^-,\mu^+) = 0 \quad \forall\, \partial z \in V, \tag{2c}$$

$$\mu^-(x), \mu^+(x) \ge 0 \text{ a.e.}, \tag{2d}$$

$$\mu^-(x)(q(x)-a) = \mu^+(x)(b-q(x)) = 0 \text{ a.e.}, \tag{2e}$$

provided that $\mathcal{L}$ is partial differentiable with respect to the variables q, u and z and the state and adjoint equation (2c) and (2b) are solvable. The multipliers μ^- and μ^+ are given as negative or positive part of

$$\alpha q - a'_q(q,u)(\cdot,z).$$

It follows from the KKT-system (2) that the control q fulfills the following (pointwise) equality:

$$q(x) = \max\Big(a, \min\Big(b, \frac{1}{\alpha}\, a'_q(q,u)(\cdot,z)\Big)\Big) \tag{3}$$

where $a'_q(q,u)(z,\cdot)$ is understood as a Riesz representative of the functional $a'_q(q,u)(z,\cdot) : L^2(\Omega) \to \mathbb{R}$.

To simplify the presentation we discretize the state and adjoint equation using continuous piecewise linear finite elements, and the control variable q is discretized using cellwise constant functions.

Then following standard arguments [3, 12] we derive the following:

Theorem 1 *Let $\chi = (q, u, z, \mu^-, \mu^+)$ be a solution to the KKT-system (2) and $\chi_h = (q_h, u_h, z_h, \mu_h^-, \mu_h^+)$ be its Galerkin approximation, then the following holds:*

$$J(q,u) - J(q_h,u_h) = \frac{1}{2}\Big(\mathcal{L}'(\chi_h)(\tilde{e}) + (\hat{e}_{\mu^-}, q-a)_{L^2} + (\hat{e}_{\mu^+}, b-q)_{L^2} + R\Big) \tag{4}$$

with a remainder term

$$R = \int_0^1 \mathcal{L}'''(\chi_h + se)(e,e,e)s(s-1)\,ds$$

and the abbreviations $e = \chi - \chi_h$, $\tilde{e} = \chi - \tilde{\chi}_h$, $\hat{e}_{\mu^-} = \hat{\mu}^- - \mu_h^-$, $\hat{e}_{\mu^+} = \hat{\mu}^+ - \mu_h^+$. With $\tilde{\chi}_h = (\tilde{q}_h, \tilde{u}_h, \tilde{z}_h, \tilde{\mu}_h^-, \tilde{\mu}_h^+)$, where $\tilde{q}_h$, $\tilde{u}_h$ and $\tilde{z}_h$ are arbitrary discrete functions, $\tilde{\mu}_h^-$ is an arbitrary discrete function whose support is contained in the set where $q_h(x) = a$ and $\tilde{\mu}_h^+$ is an arbitrary discrete function whose support is contained in the set where $q_h(x) = b$. The function $\hat{\mu}^-$ is an arbitrary L^2 function whose support is contained in the set where $q(x) = a$, and analogous for $\hat{\mu}^+$.

For the error with respect to an arbitrary functional $I : (q,u) \to \mathbb{R}$ one has to consider an auxiliary linear quadratic optimization problem for given $\chi = (q, u, z, \mu^-, \mu^+)$:

$$\min_{P^{\mathrm{ad}} \times V} K(\chi, p, v) \tag{5a}$$

$$\text{s.t. } \mathcal{L}''_{uz}(\chi)(v,\phi) + \mathcal{L}''_{qz}(\chi)(p,\phi) = 0 \quad \forall\, \phi \in V \tag{5b}$$

where the cost functional is given as

$$K(\chi,p,v) = I'_u(q,u)(v) + I'_q(q,u)(p) + \mathcal{L}''_{uq}(\chi)(v,p) + \frac{1}{2}\mathcal{L}''_{uu}(\chi)(v,v) + \frac{1}{2}\mathcal{L}''_{qq}(\chi)(p,p)$$

and the admissible set P^{ad} is defined by the lower and upper bound

$$p_-(x) = \begin{cases} 0 & \mu^+(x) - \mu^-(x) \neq 0 \text{ or} q(x) = a \\ -\infty & \text{else} \end{cases},$$

$$p_+(x) = \begin{cases} 0 & \mu^+(x) - \mu^-(x) \neq 0 \text{ or} q(x) = b \\ \infty & \text{else} \end{cases}.$$

For the discretization and the corresponding KKT-systems we refer to [12]. Then using the Lagrangian

$$\mathcal{M}(\chi, \psi) = I(q,u) + \mathcal{L}'(\chi)(\psi) :$$

one obtains an equality for the error in the the quantity of interest similar to the one in Theorem 1.

These identities can be used to obtain local indicators for mesh refinement by using cell wise integration by parts. For the state u we approximate the difference $u - \tilde{u}_h$ using a piecewise bilinear interpolant on a mesh with cell diameter $2h$ the Interpolation operator is denoted by $I_{2h}^{(2)}$ and then setting $u - \tilde{u}_h \approx I_{2h}^{(2)} u_h - u_h$.

The same is done for the variables z, v and y. Unfortunately is not appropriate for the other variables due to the following reasons:

- Such an approach is not possible for finite dimensional control occurring for example in parameter identification.
- q, μ^- and μ^+ are at most Lipschitz continuous and the dual variables p, ν^- and ν^+ are at most bounded due to the constraints imposed on those variables.

To overcome these difficulties we suggest to utilize the projection formulas, e.g, for $q - \tilde{q}_h$ we substitute

$$q - \tilde{q}_h \approx \max\Big(a, \min\Big(b, \frac{1}{\alpha}\, a_q'(q_h, I_{2h}^{(2)} u_h)(\cdot, I_{2h}^{(2)} z_h)\Big)\Big) - q_h$$

and similar but more complex formulas for the other variables. That the additional error introduced by this substitution is of higher order is indicated by superconvergence results obtained by [10].

Finaly some numerical results are shown.

References

[1] R. Becker, *Estimating the control error in the discretized PDE-constrained optimization*, J. Numer. Math., 14 (3): pp. 163–185, 2006.

[2] R. Becker, H. Kapp, R. Rannacher, *Adaptive finite element methods for optimal control of partial differential equations: Basic concepts*, SIAM J. Control Optim., 39 (1): pp. 113–132, 2000.

[3] R. Becker, R. Rannacher, *An Optimal Control Approach to A-Posteriori Error Estimation*, Acta Numerica, Cambridge University Press, pp. 1–102, 2001.

[4] R. Becker, B. Vexler, *A posteriori error estimation for finite element discretizations of parameter identification problems*, Numer. Math., 96 (3): pp. 435–459, 2004.

[5] M. Hintermüller, R.H.W. Hoppe, *Goal-oriented adaptivity in control constrained optimal control of partial differential equations*. Submitted to SIAM J. Control Optim.

[6] M. Hintermüller, R.H.W. Hoppe, Y. Iliash, M. Kieweg, *An a posteriori error analysis of adaptive finite element methods for distributed elliptic control problems with control constraints*, to appear in ESAIM Control Optim. Calc. Var., 2006.

[7] R.H.W. Hoppe, Y. Iliash, C. Iyyunni, N.H. Sweilam, *A posteriori error estimates for adaptive finite element discretizations of boundary control problems*, J. Numer. Math., 14: pp. 57–82, 2006.

[8] R. Li, W. Liu, H. Ma, T. Tang, *Adaptive finite element approximation for distributed elliptic optimal control problems*, SIAM J. Control Optim.,41 (5): pp. 1321–1349, 2002.

[9] W. Liu, N. Yan, *A posteriori error estimates for distributed convex optimal control problems*, Adv. Comput. Math., 15 (1): pp. 285–309, 2001.

[10] C. Meyer, A. Rösch, *Superconvergence properties of optimal control problems*, SIAM J. Control Optim., 43: pp. 970–985, 2004.

[11] F. Tröltzsch, *Optimale Steuerung partieller Differentialgleichungen*, Vieweg, 2005.

[12] B. Vexler, W. Wollner, *Adaptive finite elements for elliptic optimization problems with control constraints*, Preprint of DFG SPP 1253 (2007), Number: SPP1253-23-01.

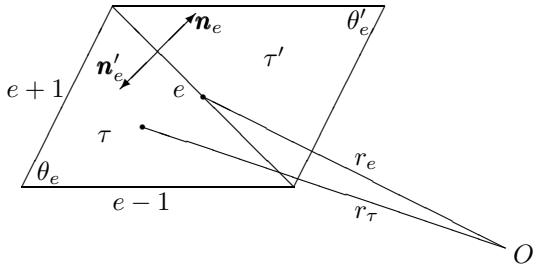
Gradient recovery and adaptive finite element methods

Zhimin Zhang

1. Introduction. While the convergence behavior of residual type error estimators is well understood, e.g., see [2, 5, 6, 7, 9, 10, 11, 15], much less is known about recovery type error estimators in theoretical aspects [14]. In this project, we study Gradient recovery techniques and their usage in adaptive finite element methods. We focus on adaptive finite element methods for elliptic problems with domain corner singularities. Our model problem is the two-dimensional Poisson equation. Results here are twofold. First, we prove that there exists an adaptive mesh (gauged by a discrete mesh density function) under which the recovered gradient by the Polynomial Preserving Recovery [19] (PPR) is superconvergent. Second, we demonstrate by numerical examples that an adaptive procedure with an *a posteriori* error estimator based on PPR does produce adaptive meshes that satisfy our mesh density assumption, and the recovered gradient by PPR is indeed superconveregent in the adaptive process [17].

Furthermore, we utilize the recovered gradient by PPR to enhance the eigenvalue approximation of the Laplace operator under adaptive meshes. Superconvergence rate is established and numerical tests on benchmark problems support our theoretical findings.

2. Mesh Conditions. We assume that O is a re-entrant corner of the domain Ω where the solution u has a leading term $r^\delta \phi(\theta)$. For a given mesh $\mathcal{M}_h$, let τ and τ' be two adjacent triangles that share a common edge e. We denote h_e the length of e, h_τ the diameter of τ, $\Omega_e = \tau \cup \tau'$ the patch of e, r_e the distance from the singular point O to the midpoint of e, and r_τ the distance from O to the barycenter of τ.



Condition (α, σ, μ): If there exist constants $\alpha > 0$, $\sigma \geq 0$, and $\mu > 0$ such that the interior edges can be separated into two parts $\mathcal{E}_h = \mathcal{E}_{1,h} \oplus \mathcal{E}_{2,h}$: Ω_e forms an $O\big(h_e^{1+\alpha}/r_e^{\alpha+\mu(1-\alpha)}\big)$ parallelogram for $e \in \mathcal{E}_{1,h}$ and the number of edges in $\mathcal{E}_{2,h}$ satisfies $\#\mathcal{E}_{2,h} \lesssim N^\sigma$, where N is the total number of degrees of freedom.

Let us elaborate on this mesh condition.

• Roughly, the edges can be grouped into "good" ($\mathcal{E}_{1,h}$) and "bad" ($\mathcal{E}_{2,h}$), where the number of bad edges are much smaller than that of good edges. The ratio is

$$\frac{\#\mathcal{E}_{2,h}}{\#\mathcal{E}_{1,h}} \lesssim \frac{N^\sigma}{N} = \frac{1}{N^{1-\sigma}}.$$

• When $r_e = O(1)$, i.e., an edge e is far away from the singular point O, the mesh condition requires that Ω_e is allowed to distort $O(h_e^{1+\alpha})$ from a parallelogram, which is the same as in previous works [12, 13, 18].

• When e is in a neighborhood of O, where $r_e^{1+\mu(1-\alpha)/\alpha} \lesssim h_e$, the condition $O(h_e)$ implies $O\big(h_e^{1+\alpha}/r_e^{\alpha+\mu(1-\alpha)}\big)$. In other words, Ω_e is allowed to distort $O(h_e)$ from a parallelogram, which imposes no restriction.

• Number of edges in $\mathcal{E}_{1,h}$ that have no restriction imposed are $O(N^{1-\alpha})$ if $h_\tau \eqsim r_\tau^{1-\mu}\underline{h}^\mu$ for any $\tau \in \mathcal{M}_h$. Here $\underline{h}$ and μ are positive constants.

• The closer we are to the singular point, the less restriction is imposed on the mesh. Indeed, for an adaptively refined mesh, the closer we are to the singular point, the worse the mesh quality is in terms of forming parallelogram triangular pairs.

3. Recovery Operators. Let V_k^h be a C^0 finite element space of degree k. Given approximation $u_h \in V_k^h$ of u, the goal is to obtain a better gradient $G_h u_h$ by some post-processing techniques based on the computed data u_h, such that

$$\|\nabla u - G_h u_h\| << \|\nabla u - \nabla u_h\|$$

Here are some popular recovery methods: 1) Simple or weighted averaging [1, 4]; 2) Local or semi-local L_2-projections [16]; 3) Zienkiewicz-Zhu Superconvergence Patch Recovery (SPR) [20, 21]; and 4) Polynomial Preserving Recovery (PPR) [12, 19].

We assume that the recovery operator G_h satisfies the following hypotheses:

a) $\|G_h v_h\|_{L^2(\Omega)} \lesssim \|\nabla v_h\|_{L^2(\Omega)}$, $\forall v_h \in V_k^h$;

b) $(G_h p)(z) = \nabla p(z)$ if $p \in P_{k+1}(\omega_z)$;

c) $|(G_h\phi)(z)| \lesssim \dfrac{1}{h_\tau} \max\limits_{z' \in \mathcal{N}_h \cap \omega_z} |\phi(z')|$;

for any nodal point $z \in \mathcal{N}_h$ and an element patch ω_z surrounding z.

4. Superconvergence Results. In the following theorem, we assume that the leading singularity term is $Kr^\delta\phi(\theta)$.

Theorem. Let $u_h \in V_k^h$ be the finite element approximation of u, the solution of the Poisson equation. Assume that a sequence of adaptive meshes $\mathcal{M}_h$ satisfy *Condition* $(\alpha, \sigma, \delta/(k+1))$ with $0 < \alpha \le 1$ and $0 \le \sigma < 1$, and that $h_\tau \eqsim r_\tau^{1-\delta/(k+1)}\underline{h}^{\delta/(k+1)}$ for any $\tau \in \mathcal{M}_h$. Then

$$\|G_h u_h - \nabla u\|_{L^2(\Omega)} \lesssim \frac{1 + (\ln N)^{1/2}}{N^{k/2+\rho}}, \quad \rho = \min(\frac{\alpha}{2}, \frac{1-\sigma}{2}).$$

Comparing with the optimal order $O(N^{-k/2})$ [5] for the adaptive methods, we see that the above theorem is a superconvergence result.

• Numerical examples indicate that an adaptive procedure with an *a posteriori* error estimator based on PPR does produce adaptive meshes that satisfy our mesh density assumption.

• The recovered gradient by PPR is indeed superconvergent in the adaptive process.

5. Eigenvalue Enhancement. In addition to the gradient recovery $G_h u_h$, we further reconstruct a new approximation w_h (different from u_h) for the eigenfunction u such that $\nabla w_h = G_h u_h$. Then we define an enhanced eigenvalue approximation

$$\lambda_h^* = \frac{\|G_h u_h\|^2_{L^2(\Omega)}}{\|w_h\|^2_{L^2(\Omega)}}.$$

Note: Usually, w_h belongs to a finite dimensional space that is larger than the original finite element space. However, we do not require $\|u - w_h\|_{L^2(\Omega)} << \|u - u_h\|_{L^2(\Omega)}$. The same order approximation $\|u - w_h\|_{L^2(\Omega)} \approx \|u - u_h\|_{L^2(\Omega)}$ would be sufficient for the eigenvalue enhancement.

The following identity by Babuška-Osborn [3] provides the error estimate

$$\frac{\|\nabla w_h\|^2_{L^2(\Omega)}}{\|w_h\|^2_{L^2(\Omega)}} - \lambda = \frac{\|\nabla(w_h - u)\|^2_{L^2(\Omega)}}{\|w_h\|^2_{L^2(\Omega)}} - \lambda \frac{\|u - w_h\|^2_{L^2(\Omega)}}{\|w_h\|^2_{L^2(\Omega)}}.$$

Recall

$$G_h u_h = \nabla w_h, \quad \|w_h - u\|_{L^2(\Omega)} = O(h^{k+1}).$$

Then

$$\lambda_h^* - \lambda = \frac{\|G_h u_h - \nabla u\|^2_{L^2(\Omega)}}{\|w_h\|^2_{L^2(\Omega)}} + O(h^{2(k+1)}).$$

Therefore, if

$$\|G_h u_h - \nabla u\|_{L^2(\Omega)} \leq C h^{k+\rho},$$

we do have the "double order" gain in the enhanced eigenvalue approximation

$$\lambda_h^* - \lambda = O(h^{2(k+\rho)}),$$

as we have observed from numerical experiments [13].

Further Extension. The recovery can be applied to general eigenvalue problems

$$a(u, v) = \lambda b(u, v),$$

where the identity

$$\lambda_h - \lambda = \|u - u_h\|^2_a - \lambda \|u - u_h\|^2_b$$

is hold.

Suggestion: Applying gradient recovery whenever it is possible.

References

[1] Ainsworth, M. and Oden, J.T., *A Posteriori Error Estimation in Finite Element Analysis*, Wiley Interscience, New York, 2000.

[2] Babgerth, W. and Rannacher, R., *Adaptive Finite Element Methods for Differential Equations*, Birkhäser, Basel, 2003.

[3] Babuška, I. and Osborn, J.E., *Eigenvalue problems*, in: *Handbook of Numerical Analysis Vol.II, Finite Element Methods* (Part I), P.G. Ciarlet and J.L. Lions, eds, Elsevier, 1991, 641-792.

[4] Babuška, I. and Strouboulis, T., *The Finite Element Method and its Reliability*, Oxford University Press, London, 2001.

[5] Binev, P., Dahmen, W., and DeVore, R., Adaptive finite elements with convergence rates, *Numer. Math.*, 97-2 (2004), 219-268.

[6] Carstensen, C. and Hoppe, R.H.W., Convergence analysis of an adaptive nonconforming finite element method, *Numer. Math.*, 103-2 (2006), 251-266.

[7] Dörfler, W., A convergent adaptive algorithm for Poisson's equation, *SIAM J. Numer. Anal.*, 33 (1996), 1106-1124.

[8] Fierro F. and Veeser, A., A posteriori error estimators, gradient recovery by averaging, and superconvergence, *Numer. Math.*, 103 (2006), 267-298.

[9] Gavaghan, D.G., Gillow, K., and Süli, E., Adaptive Finite Element Methods in Electrochemistry, *Langmuir*, Vol.22 No.25 (2006), 10666-10682.

[10] Eriksson, K., Estep, D., Hansbo, P., and Johnson, C., Adaptive methods for differential equations, Acta Numerica (1995), 1-50.

[11] Morin, P., Nochetto, R.H., and Siebert, K.G., Convergence of adaptive finite element methods, *SIAM Review*, 44-4 (2002), 631-658.

[12] Naga, A. and Zhang, Z., A posteriori error estimates based on polynomial preserving recovery, *SIAM J. Numer. Anal.*, 42-2 (2004), 1780-1800.

[13] Naga, A., Zhang, Z., and Zhou, A., Enhancing eigenvalue approximation by gradient recovery, *SIAM J. Sci. Comput*, 28-4 (2006), 1289-1300.

[14] Tang, T. and Xu, J. (eds.), *Adaptive Computations: Theory and Algorithms*, Science Press, Beijing, 2007.

[15] Verfürth, R., *A Posteriori Error Estimation and Adaptive Mesh Refinement Techniques*, Teubner Skripten zur Numerik, B.G. Teubner, Stuttpart, 1995.

[16] Wahlbin, L.R., *Superconvergence in Galerkin Finite Element Methods*, Lecture Notes in Mathematics 1605, Springer, Berlin, 1995.

[17] Wu, H. and Zhang, Z., Can we have superconvergent gradient recovery under adaptive meshes? Accepted for publication by *SIAM J. Numer. Anal.*

[18] Xu, J. and Zhang, Z., Analysis of recovery type a posteriori error estimators for mildly structured grids, *Math. Comp.*, 73 (2003), 1139-1152.

[19] Zhang, Z. and Naga, A., A new finite element gradient recovery method: Superconvergence property, *SIAM J. Sci. Comput.*, 26-4 (2005), 1192-1213.

[20] Zienkiewicz, O.C., Taylor, R.L., and Zhu, J.Z., *The Finite Element Method*, 6th ed., McGraw-Hill, London, 2005.

[21] Zienkiewicz, O.C. and Zhu, J.Z., The superconvergence patch recovery and a posteriori error estimates, Part 1: The recovery technique, *Internat. J. Numer. Methods Engrg.*, 33 (1992), 1131-1364.

Reporter: Rolf Rannacher

Participants

Prof. Dr. Mark Ainsworth
Department of Mathematics
University of Strathclyde
Livingstone Tower
26, Richmond Street
GB-Glasgow , G1 1XH

Prof. Dr. Thomas Apel
Institut für Mathematik und
Bauinformatik
Universität der Bundeswehr München
85577 Neubiberg

Prof. Dr. Wolfgang Bangerth
Department of Mathematics
Texas A & M University
College Station , TX 77843-3368
USA

Prof. Dr. Peter G. Binev
Dept. of Mathematics
University of South Carolina
Columbia , SC 29208
USA

Prof. Dr. Malte Braack
Mathematisches Seminar
Christian-Albrechts-Universität Kiel
Ludewig-Meyn-Str. 4
24118 Kiel

Prof. Dr. Carsten Carstensen
Institut für Mathematik
Humboldt-Universität zu Berlin
Unter den Linden 6
10099 Berlin

Dr. Andreas Dedner
Abteilung für Angewandte Mathematik
Universität Freiburg
Hermann-Herder-Str. 10
79104 Freiburg

Prof. Dr. Alan Demlow
Department of Mathematics
University of Kentucky
715 Patterson Office Tower
Lexington , KY 40506-0027
USA

Prof. Dr. Willy Dörfler
Institut für Angewandte Mathematik
II,
TU Karlsruhe
76128 Karlsruhe

Thomas Dunne
Institut für Angewandte Mathematik
Universität Heidelberg
Im Neuenheimer Feld 294
69120 Heidelberg

Prof. Dr. Ricardo Duran
Dto. de Matematica - FCEYN
Universidad de Buenos Aires
Ciudad Universitaria
Pabellon 1
1428 Buenos Aires
ARGENTINA

Alexandra Gaevskaya
Institut für Mathematik
Universität Augsburg
Universitätsstr. 14
86159 Augsburg

Janice Giudice
Computing Laboratory
Oxford University
8 - 11, Keble Road
GB-Oxford OX1 3QD

Elena Gorshkova
Dept. of Mathematical Information Technology
PO Box 35 (Agora)
FIN-40014 University of Jyväskylä

Prof. Dr. Wolfgang Hackbusch
Max-Planck-Institut für Mathematik in den Naturwissenschaften
Inselstr. 22 - 26
04103 Leipzig

Dr. Peter Hansbo
Department of Mathematics
Chalmers University of Technology and University of Göteborg
Sven Hultins gata 6
S-41296 Göteborg

Dr. Ralf Hartmann
DLR, Institute of Aerodynamics and Flow Technology
Numerical Methods
Lilienthalplatz 7
38108 Braunschweig

Prof. Dr. Vincent Heuveline
Institut f. Angewandte und Numerische Mathematik - Universität Karlsuhe (TH)
-Rechenzentrum-
Zirkel 2
76128 Karlsruhe

Prof. Dr. Ronald H.W. Hoppe
Lehrstuhl für Angewandte Mathematik I
Universität Augsburg
Universitätsstr. 14
86159 Augsburg

Prof. Paul Houston
School of Mathematical Sciences
University of Nottingham
University Park
GB-Nottingham NG7 2RD

Prof. Dr. Claes Johnson
Department of Mathematics
Chalmers University of Technology
S-412 96 Göteborg

Prof. Dr. Guido Kanschat
Department of Mathematics
Texas A & M University
College Station , TX 77843-3368
USA

Christian Kreuzer
Institut für Mathematik
Universität Augsburg
Universitätsstr. 14
86159 Augsburg

Prof. Dr. Angela Kunoth
Institut für Angewandte Mathematik
Universität Bonn
Wegelerstr. 6
53115 Bonn

Jason Kurtz
Institute for Computational Engineering and Sciences (ICES)
University of Texas at Austin
ACES 6.332
Austin , TX 78712-1085
USA

Prof. Dr. Jens Lang
Fachbereich Mathematik
TU Darmstadt
Schloßgartenstr. 7
64289 Darmstadt

Dr. Mats G. Larson
Dept. of Mathematics
University of Umea
S-901 87 Umea

Prof. Dr. Stig Larsson
Department of Mathematics
Chalmers University of Technology
S-412 96 Göteborg

Dr. Shipeng Mao
Institute of Computational Mathematics
Chinese Academy of Sciences
P.O.Box 2719
Beijing 100080
CHINA

Dr. Joseph Maubach
Department of Mathematics and
Computer Science
Post Box 513
NL-5600 MB Eindhoven

Dipl.-Math. Dominik Meidner
Institut für Angewandte Mathematik
Universität Heidelberg
Im Neuenheimer Feld 294
69120 Heidelberg

Prof. Dr. Jens Markus Melenk
Institut für Analysis und
Scientific Computing
Technische Universität Wien
Wiedner Hauptstr. 8 - 10
A-1040 Wien

Prof. Dr. Pedro Morin
Departamento de Matematica
IMAL
Universidad Nacional del Litoral
Güemes 3450
S 3000 GLN Santa Fe
ARGENTINA

Prof. Dr. Ricardo H. Nochetto
Department of Mathematics
University of Maryland
College Park , MD 20742-4015
USA

Christoph Ortner
Computing Laboratory
Oxford University
Wolfson Building
Parks Road
GB-Oxford OX1 3QD

Dr. Marco Picasso
Institut d'Analyse et Calcul Scientifiq.
EPFL Lausanne
SB-IACS-ASN, Bat.MA, Station 8
CH-1015 Lausanne

Dr. Serge Prudhomme
ICES
The University of Texas at Austin
1 University Station, C0200
Austin TX 78712-0027
USA

Prof. Dr. Rolf Rannacher
Institut für Angewandte Mathematik
Universität Heidelberg
Im Neuenheimer Feld 294
69120 Heidelberg

Prof. Dr. Sergey I. Repin
St. Petersburg Branch of Steklov
Mathematical Institute
Fontanka 27
191011 St. Petersburg
Russia

Prof. Dr. Kunibert G. Siebert
Institut für Mathematik
Universität Augsburg
Universitätsstr. 14
86159 Augsburg

Prof. Dr. Rob Stevenson
Department of Mathematics
Utrecht University
P.O.Box 80.010
NL-3508 TA Utrecht

Prof. Dr. Endre Süli
Computing Laboratory
Oxford University
Wolfson Building
Parks Road
GB-Oxford OX1 3QD

Prof. Dr. Franz-Theo Suttmeier
Universität Siegen
Fachbereich 6 Mathematik
Walter-Flex-Str. 3
57068 Siegen

Prof. Dr. Anders Szepessy
NADA
The Royal Institute of Technology
Department of Mathematics
S-10044 Stockholm

Prof. Dr. Andreas Veeser
Dipartimento di Matematica
Universita di Milano
Via C. Saldini, 50
I-20133 Milano

Prof. Dr. Rüdiger Verfürth
Fakultät für Mathematik
Ruhr-Universität Bochum
Universitätsstr. 150
44801 Bochum

Dr. Boris Vexler
Johann Radon Institute
Austrian Academy of Sciences
Altenberger Straße 69
A-4040 Linz

Prof. Dr. Barbara Wohlmuth
Institut für Angewandte Analysis
und Numerische Simulation
Universität Stuttgart
Pfaffenwaldring 57
70569 Stuttgart

Winnifried Wollner
Institut für Angewandte Mathematik
Universität Heidelberg
Im Neuenheimer Feld 294
69120 Heidelberg

Prof. Dr. Zhimin Zhang
Department of Mathematics
College of Science and Liberal Arts
Wayne State University
Detroit , MI 48202
USA