

MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

Report No. 42/2016

DOI: 10.4171/OWR/2016/42

Self-Adaptive Numerical Methods for Computationally Challenging Problems

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4 September – 10 September 2016

ABSTRACT. Self-adaptive numerical methods provide a powerful and automatic approach in scientific computing. In particular, Adaptive Mesh Refinement (AMR) algorithms have been widely used in computational science and engineering and have become a necessary tool in computer simulations of complex natural and engineering problems. The key ingredient for success of self-adaptive numerical methods is *a posteriori* error estimates that are able to accurately locate sources of global and local error in the current approximation. The workshop creates a forum for junior and senior researchers in numerical analysis and computational science and engineering to discuss recent advances, initiates future research projects, and establishes new collaborations on convergence theory of adaptive numerical methods and on the construction and analysis of efficient, reliable, and robust *a posteriori* error estimators for computationally challenging problems.

Mathematics Subject Classification (2010): 65-XX, 65Mxx, 65Nxx, 73Vxx, 76Mxx.

Introduction by the Organisers

The workshop was organized by Randolph E. Bank (UCSD, La Jolla), Zhiqiang Cai (Purdue, West Lafayette) and Rüdiger Verfürth (RUB, Bochum). Fifty scientists from around the world attended the workshop, held 4–10 September, 2016.

Computer simulations of complex physical, biological, and human-engineered systems exhibit a grand challenge in computational mathematics. Computational difficulties for those systems include, but are not limited to, interface singularities, discontinuities (in the form of shock-like fronts, and of interior and boundary layers), oscillations of various scales (multiscale phenomena), and high nonlinearity.

(Problems exhibiting these phenomena are referred to as computationally challenging in this proposal.) Moreover, unlike simple systems, for complex systems, there may be limited or nonexistent *a priori* knowledge of locations and properties of these phenomena that might be used for designing efficient and effective numerical algorithms.

Self-adaptive numerical methods provide a powerful and automatic approach to scientific computing. In particular, Adaptive Mesh Refinement (AMR) algorithms have been widely used in computational science and engineering and have become a necessary tool in computer simulations of complex natural and engineering problems. As identified by the US National Research Council, AMR is one of two necessary tools for computationally grand challenge problems. The key ingredient for success of AMR algorithms is *a posteriori* error estimates that are able to accurately locate sources of global and local error in the current approximation.

Another challenge in computer simulations of complex systems is reliability of computer predictions. Mathematically speaking, this means robust and accurate estimates of the error in the computed numerical solution of the underlying problem. *A priori* error estimates, as provided, e.g., by the standard error analysis for finite element, finite volume, or finite difference methods, are often insufficient since they only yield information on the asymptotic error behavior. Moreover, stability and regularity estimates needed for *a priori* error estimates typically are not available for complex systems.

These considerations (error control, efficiency in AMR algorithms, etc.) demonstrate the need for an error estimator that can *a posteriori* be extracted from the computed numerical solution and the given data of the underlying problem. Such an *a posteriori* error estimate ideally should provide an underlying rigorous mathematical theory for estimating and quantifying discretization error in terms of the error's magnitude and its spacial distribution.

Presentations covered a wide range of topics, among them

- Adaptive Multiscale Methods
- Adaptive Model Reduction
- Space-Time Adaptivity for Evolution Equations
- Parallel Adaptive Multigrid Solvers
- A Posteriori Error Estimation
- Optimality of Certain AFEM algorithms
- Adaptive Approaches for Applications of Scientific and Engineering Interest

Acknowledgement: The MFO and the workshop organizers would like to thank the National Science Foundation for supporting the participation of junior researchers in the workshop by the grant DMS-1049268, "US Junior Oberwolfach Fellows". Moreover, the MFO and the workshop organizers would like to thank the Simons Foundation for supporting James Brannick in the "Simons Visiting Professors" program at the MFO.

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Abstracts

An analysis of multiscale methods based on subspace decomposition

HARRY YSERENTANT

(joint work with Ralf Kornhuber, based on results of Daniel Peterseim)

Numerical homogenization tries to approximate the solutions of elliptic partial differential equations with strongly oscillating coefficients by functions from modified finite element spaces. I presented in this talk a class of such methods that are very closely related to the method of Målqvist and Peterseim [2], [3]. Like the method of Målqvist and Peterseim, the new methods do not make explicit or implicit use of a scale separation. Their comparatively simple analysis is based on the theory of additive Schwarz or subspace decomposition methods.

The model problem under consideration is a linear second order differential equation in weak form with homogeneous Dirichlet boundary conditions on a polygonal domain Ω . Its solution space is the Sobolev space $H_0^1(\Omega)$ and the associated bilinear form reads

$$(1) \quad a(u, v) = \int_{\Omega} \nabla u \cdot A \nabla v \, dx.$$

The matrix A is a function of the spatial variable x with measurable entries and assumed to be symmetric positive definite. We assume that

$$(2) \quad \delta |\eta|^2 \leq \eta \cdot A(x) \eta \leq M |\eta|^2$$

holds for all $\eta \in \mathbb{R}^d$ and almost all $x \in \Omega$, where $|\eta|$ denotes the euclidian norm of η and δ and M are positive constants. The Lax-Milgram theorem states under this condition that the boundary value problem

$$(3) \quad a(u, v) = \int_{\Omega} f v \, dx, \quad v \in H_0^1(\Omega),$$

possesses for all $f \in L_2(\Omega)$ a unique solution $u \in H_0^1(\Omega)$.

The key ingredient of the methods is a bounded local linear projection operator

$$(4) \quad \Pi : H_0^1(\Omega) \rightarrow \mathcal{S} : u \rightarrow \Pi u$$

from the solution space to a first-order, conforming finite element space \mathcal{S} , like that defined as follows. At first, the given function $u \in H_0^1(\Omega)$ is locally, on the single elements, approximated by its L_2 -orthogonal projection onto the space of linear functions, without regard to the continuity across the boundaries of the elements. In a second step, the values of these approximants at a vertex in the interior of the domain are replaced by their arithmetic mean and their values at a vertex on the boundary by the value zero. These values characterize and fix the projection Πu of u onto \mathcal{S} . For the functions u in the solution space $H_0^1(\Omega)$, then the estimates

$$(5) \quad |\Pi u|_1 \leq c_1 |u|_1, \quad \|h^{-1}(u - \Pi u)\|_0 \leq c_2 |u|_1$$

hold, where $\|\cdot\|_0$ denotes the L_2 -norm, $|\cdot|_1$ the H^1 -seminorm, and h is an elementwise constant function whose value on the interior of a given element is its

diameter. The first condition means that the projection operator (4) is stable with respect to the H^1 -norm and therefore, by condition (2), also with respect to the energy norm $\|\cdot\|$ induced by the bilinear form (1) underlying the boundary value problem. The second condition is an approximation property.

The kernel \mathcal{V} of Π is a closed subspace of $H_0^1(\Omega)$ and therefore itself a Hilbert space. Thus we can introduce the a -orthogonal projection operator C from $H_0^1(\Omega)$ onto the kernel of Π and moreover the finite dimensional subspace

$$(6) \quad \mathcal{W} = \{v - Cv \mid v \in \mathcal{S}\}$$

of the a -orthogonal complement of the kernel of Π . The dimension of \mathcal{W} and of the finite element space \mathcal{S} coincide as $v \in \mathcal{S}$ can be recovered from $v - Cv$ via

$$(7) \quad v = \Pi(v - Cv).$$

Målqvist and Peterseim [2], [3] discretize the equation (3) using \mathcal{W} both as trial and test space. Starting point of our theory is Peterseim's observation that the approximate solution $w \in \mathcal{W}$, the a -orthogonal projection of the exact solution $u \in H_0^1(\omega)$ of the equation onto \mathcal{W} , possesses the representation

$$(8) \quad w = \Pi u - C\Pi u$$

and that the error $u - w = Cu$ is the a -orthogonal projection of the solution onto the kernel \mathcal{V} of Π . This implies the estimate

$$(9) \quad \|u - w\| \leq c \|hf\|_0$$

of the energy norm error [2]. Remarkably, neither the smoothness of the solution nor the regularity properties of the equation enter into the constant. The size of the error is determined by the local behavior of the right hand side f .

Let x_1, x_2, \dots, x_n be the vertices of the elements in the triangulation underlying the finite element space \mathcal{S} and let $\varphi_1, \varphi_2, \dots, \varphi_n$ be the piecewise linear hat functions assigned to these nodes. The φ_i assigned to the nodes in the interior of the domain Ω form then a basis of the finite element space \mathcal{S} , and the corresponding functions $\varphi_i - C\varphi_i$ a basis of the trial space (6). Målqvist and Peterseim [2] have shown that these basis functions decay exponentially with the distance to the assigned nodes and can therefore be replaced by localized counterparts. We utilize the theory of iterative methods to prove a result of similar kind [1]. Let ω_i be the union of the finite elements with vertex x_i , the support of φ_i , and let

$$(10) \quad \mathcal{V}_i = \{v - \Pi v \mid v \in H_0^1(\omega_i)\}.$$

The functions in \mathcal{V}_i vanish outside a small neighborhood of the vertex x_i , depending on the choice of Π . The \mathcal{V}_i are closed subspaces of the kernel \mathcal{V} of Π . Let P_i be the a -orthogonal projection from $H_0^1(\Omega)$ to \mathcal{V}_i , defined via the equation

$$(11) \quad a(P_i v, v_i) = a(v, v_i), \quad v_i \in \mathcal{V}_i.$$

Introducing the operator

$$(12) \quad T = P_1 + P_2 + \dots + P_n,$$

the approximation spaces replacing \mathcal{W} are built up with the help of the bounded linear operators F_ν from $H_0^1(\Omega)$ to \mathcal{V} that are, starting from $F_0u = 0$, defined via

$$(13) \quad F_{\nu+1}u = F_\nu u + T(u - F_\nu u).$$

The correction $T(u - F_\nu u)$ is the sum of its components $d_i = P_i(u - F_\nu u)$ in the subspaces \mathcal{V}_i of \mathcal{V} , the solutions $d_i \in \mathcal{V}_i$ of the local equations

$$(14) \quad a(d_i, v_i) = a(u, v_i) - a(F_\nu u, v_i), \quad v_i \in \mathcal{V}_i.$$

The new trial and test spaces are the spaces \mathcal{W}_ℓ spanned by the functions

$$(15) \quad \varphi_i - F_\nu \varphi_i, \quad \nu = 0, 1, \dots, \ell,$$

attached to the nodes x_i in the interior of the domain Ω . In contrast to their counterparts $\varphi_i - C\varphi_i$ spanning the original space \mathcal{W} they have a local support, which expands layer by layer with the number ν of iterations.

To study the approximation properties of these spaces \mathcal{W}_ℓ , we consider optimally chosen fixed linear combinations

$$(16) \quad C_\ell = \sum_{\nu=0}^{\ell} \alpha_{\ell\nu} F_\nu, \quad \sum_{\nu=0}^{\ell} \alpha_{\ell\nu} = 1,$$

of the operators F_ν as approximations of the a -orthogonal projection C . These operators C_ℓ serve solely as a tool and do not need to be explicitly accessible. Our analysis starts from the observation that, for all $v \in \mathcal{V}$, there is a with respect to the energy norm stable decomposition $v = v_1 + \dots + v_n$ of v into functions v_i in the local spaces \mathcal{V}_i , such that

$$(17) \quad \sum_{i=1}^n \|v_i\|^2 \leq K_1 \|v\|^2$$

holds. Moreover, there is a constant K_2 such that

$$(18) \quad \|v\|^2 \leq K_2 \sum_{i=1}^n \|v_i\|^2$$

holds for all such decompositions of v into functions v_i in the subspaces \mathcal{V}_i of the kernel. The proof of the first estimate utilizes the properties (5) of the projection Π , and therefore in particular that the functions v in the kernel \mathcal{V} of Π are rapidly oscillating, and the assumption (2) on the coefficient functions. The constant in the second estimate can be bounded in terms of the maximum number of the parts v_i that do not vanish on a given element.

The operator T maps the kernel \mathcal{V} to itself and can be considered as a bounded, symmetric operator from \mathcal{V} to \mathcal{V} . With the help of the estimates (17) and (18) one can show that its spectrum is a compact subset of the interval with the two endpoints $1/K_1$ and K_2 . Because $I - F_\nu = (I - T)^\nu$ and $F_\nu C = F_\nu$,

$$(19) \quad C - C_\ell = \left\{ \sum_{\nu=0}^{\ell} \alpha_{\ell\nu} (I - T)^\nu \right\} C.$$

Using the spectral mapping theorem and the fact that the norm of a bounded, symmetric operator from a Hilbert space to itself is equal to its spectral radius, one gets therefore, similarly to the finite dimensional case, the error estimate

$$(20) \quad \|Cu - C_\ell u\| \leq \frac{2q^\ell}{1+q^{2\ell}} \|Cu\|, \quad u \in H_0^1(\Omega),$$

where the convergence rate

$$(21) \quad q = \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}$$

is determined by the condition number $\kappa \leq K_1 K_2$ of the operator (12) seen as bounded, symmetric operator from the subspace \mathcal{V} of $H_0^1(\Omega)$ to itself. From there, it is only a small step to our final result. Let w and w_ℓ be the best approximations of the solution u of the original equation (3) in \mathcal{W} and \mathcal{W}_ℓ , respectively, with respect to the energy norm. As $\|u - w_\ell\| \leq \|u - (\Pi u - C_\ell \Pi u)\|$ and because of the representation (8) of the best approximation w in \mathcal{W} , then

$$(22) \quad \|u - w_\ell\| \leq \left(1 + \frac{2q^\ell}{1+q^{2\ell}}\right) \|u - w\| + \frac{2q^\ell}{1+q^{2\ell}} \|u - \Pi u\|.$$

We conclude that logarithmically many iteration steps ν or even less, depending on the behavior of the energy norm of $u - \Pi u$, suffice to reach the same level of accuracy as with the original space \mathcal{W} based on the exact projection C . Finally, the infinite dimensional subspaces \mathcal{V}_i of the kernel of the projection Π are replaced by discrete counterparts to obtain a computationally feasible method.

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Adaptive Localized Model Reduction

MARIO OHLBERGER

(joint work with Stephan Rave, Felix Schindler)

Many physical, chemical, biological or technical processes can be described by means of partial differential equations. Due to nonlinear dynamics, interacting processes on different scales, and possible parametric or stochastic dependencies, an analysis and prediction of the complex behavior is often only possible – if at all – with severe simplifications. This is in particular true if not only single forward problems are considered, but beyond that uncertainty quantification, parameter estimation or optimization in engineering applications are investigated.

It has been proven that modern algorithmic approaches such as higher order adaptive modeling and model order reduction combined with efficient software design for highly parallel environments outperforms the pure gain of increasing compute power. Hence, there is a need for algorithmic improvement, both concerning a reduction of the overall computational complexity and concerning new parallelization paradigms in order to exploit the computational resources of nowadays computer architectures in an optimal manner.

A mathematical key ingredient to achieve "optimal" numerical methods is error control via rigorous a posteriori error estimates. Such error estimates can not only be used to certify approximate solutions, but rather are the essential building block in the construction of problem adapted optimal solution spaces and related adaptive numerical methods. Examples of such optimal methods are e.g. particularly tuned mesh-adaptive finite element schemes for the approximation of PDEs or reduced basis methods (weak greedy algorithms) for the approximation of parameterized PDEs.

As a particular example we investigate model reduction for spatially resolved Li-ion batteries [14] based on POD basis construction for the state space reduction and empirical interpolation [2, 4] to deal with the non-linear electrochemical reaction kinetics. Numerical experiments demonstrate a speedup of the online computational complexity with respect to the underlying finite volume approximation by a factor of about 280. In that sense the reduced basis approach is very efficient. On the other hand, this online efficiency comes with the price of an enormous offline complexity, both with respect to CPU time and with respect to storage requirements. These observations motivate the development of new model reduction paradigms that overcome the classical offline/online splitting of projection based model reduction technique. An attempt towards this goal is the development of localized model reduction methods, such as e.g. the reduced basis element method [11], the reduced basis hybrid method [7], the port reduced static condensation reduced basis element method [17], or ArbiLoMod, a new approach for handling problems with arbitrary local modifications [3].

In this contribution we focus on the localized reduced basis methods (LRBM), which were first introduced in the context of elliptic heterogeneous multiscale problems in [9] and later applied in the context of two phase flow in porous media in [8]. As demonstrated in [1], such an approach has the potential to reduce the offline cost at the price of a decreased online efficiency. It was also shown that depending on the choice of the macro mesh for the localization, the resulting localized reduced basis method can be seen as an interpolation of a classical reduced basis method and a Discontinuous Galerkin approximation on the underlying fine grid. First results for an application of LRBM to the fully non-linear Li-ion battery model were given in [13]. Although this approach allowed for balancing of offline and online complexity, it still maintained the paradigm of offline/online splitting.

In a more recent approach [16] we overcome this paradigm by allowing for local basis enrichment in the online-phase. Within this new conceptual approach we do

not aim at first constructing a reduced basis that has good approximation properties with respect to the whole solution manifold of the parameterized system and then using it for fast online evaluations. We rather think of an iterative enrichment procedure, where the reduced space is updated during the online phase in an appropriate manner, while the user explores the solution manifold. To achieve this goal we allow for carefully selected adaptive local problem solves in the online phase, based on localized a posteriori error estimation. To this end, we derive robust and efficient a posteriori error estimates for the localized reduced basis approximation against the true solution of the underlying PDE. The a posteriori error estimate is based on conservative flux reconstruction for elliptic equations, following the approach in [5] and on the additional usage of elliptic reconstructions in the case of parabolic problems [6, 15]. Several numerical experiments for elliptic and parabolic applications demonstrate the applicability of the approach.

The numerical results were obtained with the newly developed model reduction algorithms implemented in the open-source Python software package pyMOR (see <http://pymor.org> and [12]).

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Spectral Upscaling for Graph Laplacian Problems in Mixed Form with Application to Finite Volume Schemes

PANAYOT S. VASSILEVSKI

(joint work with Andrew T. Barker and Chak S. Lee)

Spectral coarsening procedures for graph Laplacian problems formulated in a mixed saddle-point form are proposed in [3]. Here we give a brief (partial) summary of these results.

Given a set of positive weights $\{k_e\}_{e \in E}$ and an undirected graph G with a set of n vertices V and a set of edges $E = \{e = (i, j), i, j \in V\} \subset V \times V$, the (weighted) graph Laplacian operator \mathcal{L} is defined as

$$\mathcal{L} = \sum_{e \in E} k_e \mathbf{d}_e \mathbf{d}_e^T,$$

where the only nonzero entries of $\mathbf{d}_e \in \mathbb{R}^n$, $e = (i, j)$, are 1 and -1 , respectively at positions i and j . For $\mathbf{f} \in \mathbb{R}^n$ such that $\mathbf{1}^T \mathbf{f} = 0$, the problem $\mathcal{L} \mathbf{u} = \mathbf{f}$ can equivalently be formulated as

$$(1) \quad \begin{bmatrix} M & D^T \\ D & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{\sigma} \\ \mathbf{u} \end{bmatrix} = \begin{bmatrix} 0 \\ -\mathbf{f} \end{bmatrix}.$$

where $D = [\dots, \mathbf{d}_e, \dots]$, and $M = \text{diag}(k_e^{-1})_{e \in E}$ both act on edge-based vector $\boldsymbol{\sigma} = (\sigma_e)_{e \in E}$. The goal is to systematically produce a low-dimensional coarse model of (1) that approximates the original problem reasonably well.

The work in [3] extends the previously developed ([4]) aggregation-based coarsening procedures applied to both unknowns to allow here more than one coarse vertex degree of freedom (dof) per aggregate. These coarse dofs are selected as certain eigenvectors of local graph Laplacians associated with each aggregate. Additionally, the edge dofs are coarsened by using traces of the discrete gradients of the already constructed coarse vertex dofs. These traces are defined on the interface edges that connect any two adjacent aggregates. The overall procedure is a modification of the spectral upscaling procedure developed in [2] for the mixed

finite element problems. Approximation property of the resulting coarse space \mathbf{U}_c for vertex dofs is established, and it is shown that there are two locally constructed projections $\pi^\sigma : \Sigma \rightarrow \Sigma_c$ and $\pi^u : \mathbf{U} \rightarrow \mathbf{U}_c$, satisfying the important commutativity relation

$$D\pi^\sigma = \pi^u D.$$

The latter, as is well-known, implies the inf-sup stability of the coarse problem.

Several numerical examples on some general unstructured graphs are demonstrated in [3]. In addition, as a main application, the proposed method is applied to construct consistent and accurate coarse-scale models in reservoir simulation problems by treating a finite volume discretization (two-point flux approximation) as a graph Laplacian. In particular, the effectiveness of the proposed coarsening method on the top 35 layers of the SPE10 model [1] is illustrated below (see Figure 1). The original $60 \times 220 \times 35$ fine grid is partitioned uniformly into a

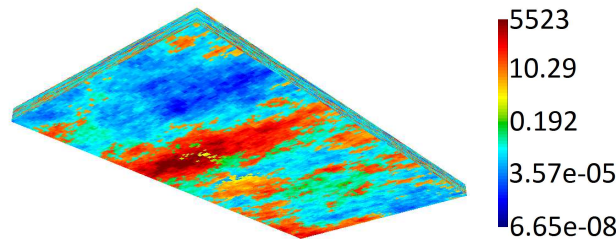
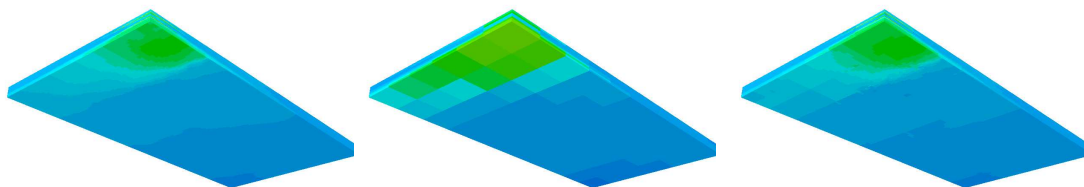


FIGURE 1. Top 35 layers of the SPE10 model.

$6 \times 11 \times 7$ coarse grid. From left to right, Figure 2 shows the pressure solution of the fine-grid reference solution, the coarse-grid solutions produced by the proposed coarsening method with number of local spectral basis $m = 1$ and 13. The relative errors (measured in l_2 norm) of the coarse-grid solutions are respectively 83.6% and 11.4%. Notice that the dimension of the fine-grid model is more than 70 times the dimension of the coarse-grid model. Both the solution plot and the error measurement show that the enriched coarse-grid solution ($m=13$) is a reliable approximation to the reference solution.



(a) Reference (dim=462000) (b) Coarse sol'n (dim=462) (c) Coarse sol'n (dim=6006)

FIGURE 2. Pressure solution plots.

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A Locally Conservative Enriched Galerkin Approximation for Flow and Transport

MARY F. WHEELER

(joint work with Sanghyun Lee, Young-Ju Lee)

Miscible displacement of one fluid by another in a porous medium has attracted considerable attention in subsurface modeling with emphasis on enhanced oil recovery applications. Here flow instabilities arising when a fluid with higher mobility displaces another fluid with lower mobility is referred to as viscous fingering. The latter has been the topic of major physical and mathematical studies for over half a century. Recently, viscous fingering has been applied for proppant-filled hydraulic fracture propagation to efficiently transport the proppant to the tip of fractures. The governing mathematical system that represents the displacement of the fluid mixtures consists of pressure, velocity, and concentration.

Here we present a novel approach to the simulation of miscible displacement by employing an adaptive enriched Galerkin finite element methods (EG) coupled with entropy residual stabilization for transport. EG is formulated by enriching the conforming continuous Galerkin finite element method (CG) with piecewise constant functions. EG provides locally and globally conservative fluxes, which is crucial for coupled flow and transport problems. Moreover, EG has fewer degrees of freedom in comparison with discontinuous Galerkin (DG) and an efficient flow solver has been derived which allows for higher order schemes. We have shown theoretically and computationally that a robust preconditioner can be achieved if one adds pre- and post smoothings to a block preconditioner involving CG and jumps in the discontinuous piecewise constants. Dynamic adaptive mesh refinement is applied in treating geological material discontinuities.

An additional advantage of EG is that only those subdomains that require local conservation need to be enriched with a treatment of high order non-matching grids. Our high-order EG transport system is coupled with an entropy viscosity residual stabilization method to avoid spurious oscillations near shocks. Instead of using limiters and non-oscillatory reconstructions, this method employs the local residual of an entropy equation to construct the numerical diffusion, which

is added as a nonlinear dissipation to the numerical discretization of the system. The amount of numerical diffusion added is proportional to the computed entropy residual. This technique is independent of mesh and order of approximation and has been shown to be efficient and stable in solving many physical problems with CG. Finally, we note that it is crucial to have dynamic mesh adaptivity in order to reduce computational costs for large-scale three-dimensional applications; both for flow and transport. We employ the entropy residual for dynamic adaptive mesh refinement to capture the moving interface between the miscible fluids. Our computational results indicate that the entropy residual can be used as an efficient posteriori error indicator.

For theoretical and computational details regarding EG for flow and transport the reader is referred to the following papers [1, 2].

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A high order trace FEM for PDEs on (evolving) surfaces

ARNOLD REUSKEN

(joint work with J. Grande, C. Lehrenfeld, M. Olshanskii)

We consider two model PDEs, namely the Laplace-Beltrami equation on a *stationary* surface a parabolic transport equation on an *evolving* surface. Given $f \in H^{-1}(\Gamma)$, with $f(1) = 0$ the Laplace-Beltrami problem is as follows: Find $u \in H_*^1(\Gamma) := \{v \in H^1(\Gamma) \mid \int_{\Gamma} v ds = 0\}$ such that

$$(1) \quad a(u, v) = f(v) \quad \text{for all } v \in H_*^1(\Gamma)$$

with

$$a(u, v) = \int_{\Gamma} \nabla_{\Gamma} u \cdot \nabla_{\Gamma} v ds.$$

The time-dependent model transport problem that we consider is as follows. Assume a surface $\Gamma(t)$ passively advected by a *given* smooth velocity field $\mathbf{w} = \mathbf{w}(x, t)$, i.e. the normal velocity of $\Gamma(t)$ is given by $\mathbf{w} \cdot \mathbf{n}$, with \mathbf{n} the unit normal on $\Gamma(t)$. We assume that for all $t \in [0, T]$, $\Gamma(t)$ is a hypersurface that is closed ($\partial\Gamma = \emptyset$), connected, oriented, and contained in a fixed domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$. The convection-diffusion equation on the surface that we consider is given by:

$$(2) \quad \dot{u} + (\operatorname{div}_{\Gamma} \mathbf{w})u - \alpha_d \Delta_{\Gamma} u = f \quad \text{on } \Gamma(t), \quad t \in (0, T],$$

with a prescribed source term $f = f(x, t)$ and homogeneous initial condition $u(x, 0) = u_0(x) = 0$ for $x \in \Gamma_0 := \Gamma(0)$. Here $\dot{u} = \frac{\partial u}{\partial t} + \mathbf{w} \cdot \nabla u$ denotes the material derivative, $\operatorname{div}_{\Gamma}$ is the surface divergence and $\alpha_d > 0$ is the constant diffusion coefficient.

In the past decade several finite element techniques for the discretization of such (elliptic and parabolic) PDEs on a smooth (evolving) surface have been developed. For a recent overview we refer to [1]. These methods can be classified as follows. Firstly, the (evolving) *surface finite element method* (SFEM), developed by Dziuk and Elliott in a series of papers (cf. [1]), is based on an explicit triangulation Γ_h of Γ . On this triangulation one uses a standard linear finite element space. In case of an evolving surface the vertices of the triangulation are transported with an interpolation of the surface velocity field. Thus this method is based on a Lagrangian approach. A second class of methods is based on an *extension of the PDE* (given on Γ) to a neighborhood of the surface. One then obtains a PDE in the volume, which can be discretized by standard FE techniques. The third class of methods consists of so-called *trace FEM* [3, 4, 5] in which one starts from a standard finite element space on an outer fixed volume mesh and then takes the trace on Γ of this space for the discretization of the surface PDE. This technique can also be applied to an evolving surface and results in a purely Eulerian approach. In this presentation we restrict to the latter class of FE trace techniques.

In the presentation, both for the case of a stationary and an evolving surface, we explain these trace finite element techniques, discuss optimal theoretical error bounds and present results of a few numerical experiments, which illustrate the behavior of the methods. For the case of a stationary interface, a very recent new result from [2] is presented. In that preprint we introduce a new *higher order* trace FEM for the Laplace-Beltrami equation. We outline the main idea. We assume that the smooth interface Γ is the zero level of a smooth level set function ϕ , i.e., $\Gamma = \{x \in \Omega \mid \phi(x) = 0\}$. The key idea is to construct a suitable *isoparametric mapping* Θ_h . For this we assume that we have available $\phi_h \in V_h^k$ (degree k standard FE space on volume triangulation) and $\hat{\phi}_h = I_1 \phi_h$ (linear interpolation), which are finite element approximations of ϕ (in a neighborhood of Γ). These finite element functions are used as input for the isoparametric mapping Θ_h . The piecewise linear surface approximation, which is easy to construct, is denoted by $\Gamma^{\text{lin}} = \{\hat{\phi}_h = 0\}$. The local volume triangulation is denoted by $\mathcal{T}^\Gamma := \{T \in \mathcal{T}, T \cap \Gamma^{\text{lin}} \neq \emptyset\}$ and the corresponding domain by Ω^Γ . The standard affine polynomial finite element space V_h^k is restricted to \mathcal{T}^Γ , i.e., $(V_h^k)|_{\Omega^\Gamma}$. To this space we apply the transformation Θ_h , resulting in the isoparametric space

$$(3) \quad V_{h,\Theta}^k := \{v_h \circ \Theta_h^{-1} \mid v_h \in (V_h^k)|_{\Omega^\Gamma}\}.$$

The unfitted finite element space that we use is the trace of this space:

$$(4) \quad V_{h,\Theta}^\Gamma := \text{tr}|_{\Gamma_h}(V_{h,\Theta}^k), \quad V_{h,\Theta}^{\Gamma,0} := \{v_h \in V_{h,\Theta}^\Gamma \mid \int_{\Gamma_h} v_h \, ds = 0\},$$

with $\Gamma_h := \Theta_h(\Gamma^{\text{lin}})$. In the notation, we skip the polynomial degree k , and we use Γ to indicate that we *take the trace of the outer volume isoparametric space*. We introduce the bilinear form

$$(5) \quad a_h(u, v) := \int_{\Gamma_h} \nabla_{\Gamma_h} u \cdot \nabla_{\Gamma_h} v \, ds.$$

For the discrete problem we need a suitable extension of the data f to Γ_h , which is denoted by f_h . The discrete problem is as follows: Find $u_h \in V_{h,\Theta}^{\Gamma,0}$ such that

$$(6) \quad a_h(u_h, v_h) = \int_{\Gamma_h} f_h v_h \, dx \quad \text{for all } v_h \in V_{h,\Theta}^{\Gamma,0}.$$

For this discretization, which is easy to implement (requires quadrature only on Γ^{lin}), optimal error bounds can be derived. An example of such a result is the following, in which δ_f is a certain data error quantity that measures the quality of the approximation $f_h \approx f$, and u^e a natural extension of u :

Theorem. *Let $u \in H^{k+1}(\Gamma)$ be the solution of (1) and $u_h \in V_{h,\Theta}^{\Gamma,0}$ the solution of (6). Assume that the data error satisfies $\|\delta_f\|_{L^2(\Gamma_h)} \leq ch^{k+1}\|f\|_{L^2(\Gamma)}$. Then the following holds:*

$$(7) \quad \|u^e - u_h\|_{H^1(\Gamma_h)} \leq ch^k \|u\|_{H^{k+1}(\Gamma)} + h^{k+1} \|f\|_{L^2(\Gamma)}.$$

Results of numerical experiments are presented which illustrate the higher order convergence of this new method.

The results presented in this talk are based on [2, 3, 4, 5].

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An adaptive space-time discontinuous Galerkin method for linear hyperbolic systems

WILLY DÖRFLER

(joint work with Stefan Findeisen, Christian Wieners)

A space-time setting for linear hyperbolic operators. We consider linear hyperbolic systems of conservation laws on a bounded domain $\Omega \subset \mathbb{R}^d$ and for some time $T > 0$,

$$Lu = f \quad \text{on } Q := \Omega \times (0, T), \quad u(\cdot, 0) = u_0,$$

where $u : Q \rightarrow \mathbb{R}^J$ and

$$Lu := M\partial_t u + Au = M\partial_t u + \nabla \cdot F(u)$$

for some bounded and positive symmetric matrix-valued function $M \in \mathbb{R}^{J,J}$ and smooth $F : \mathbb{R}^J \rightarrow \mathbb{R}^{J,d}$. We then let $W := L_2(Q)^J$ with

$$\|w\|_W := (Mw, w)_{L_2(Q)^J}^{1/2} = \|M^{1/2}w\|_{L_2(Q)^J}$$

and $V := \text{dom}(L) \subset L_2(Q)^J$ with

$$\|v\|_V := (\|v\|_W^2 + (M^{-1}Lv, Lv)_{L_2(Q)^J})^{1/2}.$$

A is assumed to be nonnegative, i. e., $(Av, v)_{L_2(Q)^J} \geq 0$ for all $v \in V$.

The variational problem on $V \times W$ is easily treated with the standard Babushka setting [2, Thm. III.3.6].

Theorem 1. [3, Thm. 2] *For given $f \in L_2(Q)^J$ there exists a unique solution $u \in V$ of*

$$(1) \quad (Lu, w)_{L_2(Q)^J} = (f, w)_{L_2(Q)^J} \quad \text{for all } w \in W$$

satisfying the a priori bound $\|u\|_V \leq \sqrt{4T^2 + 1} \|M^{-1/2}f\|_{L_2(Q)^J}$.

A space-time discontinuous Galerkin discretisation. Let Ω be decomposed into simplices K and $[0, T]$ into intervals I , we define a space-time discretisation into prisms $R = K \times I$ by $\mathcal{R} = \cup\{R\} = \cup\{K \times I\}$. We let V_h be the space of functions that are piecewise polynomials in $(\mathbb{P}_{p_K}(K) \otimes \mathbb{P}_{q_K}(I))^J$ on $R = K \times I$, discontinuous in space but continuous in time. Correspondingly, W_h is the space of piecewise polynomials in $(\mathbb{P}_{p_K}(K) \otimes \mathbb{P}_{q_K-1}(I))^J$, discontinuous in space and time.

We approximate the operator A using the nodal discontinuous Galerkin method [4]. Choosing a numerical flux function F^{num} we define $A_h v_h \in W_h$ for $v_h \in V_h$ by

$$\begin{aligned} (A_h v_h, w_h)_{L_2(Q)^J} = & \sum_{R=K \times I \in \mathcal{R}} \left\{ (\nabla \cdot F(v_{h,R}), w_{h,R})_{L_2(R)^J} \right. \\ & \left. + \sum_{f \in \mathcal{F}_K} (n_K \cdot (F_K^{\text{num}}(v_h) - F(v_{h,R})), w_{h,R})_{L_2(f \times I)^J} \right\} \end{aligned}$$

for all $w_h \in W_h$. For any simplex K , n_K denotes its exterior normal, \mathcal{F}_K the set of its faces K , and $v_{h,R}, w_{h,R}$ denotes restriction to R . We now define the discrete space-time operator L_h by $(L_h v_h, w_h)_{L_2(Q)^J} = (M_h \partial_t v_h + A_h v_h, w_h)_{L_2(Q)^J}$.

For the described space-time discretisation we can achieve existence and convergence of discrete solutions.

Theorem 2. [3, Thm. 4] *For given $f \in L_2(Q)^J$ there exists a unique solution $u_h \in V_h$ of*

$$(2) \quad (L_h u_h, w_h)_{L_2(Q)^J} = (f, w_h)_{L_2(Q)^J} \quad \text{for all } w_h \in W_h,$$

satisfying the a priori bound $\|u_h\|_{V_h} \leq \sqrt{4T^2 + 1} \|M_h^{-1} \Pi_h f\|_W$.

Theorem 3. [3, Thm. 5] *Let $u \in V$ be the solution of (1) and $u_h \in V_h$ the solution of (2). Then, we have*

$$\|u - u_h\|_{V_h} \leq (1 + \sqrt{4T^2 + 1}) \inf_{v_h \in V_h} \|u - v_h\|_{V_h}.$$

If in addition the solution is sufficiently smooth, we obtain the a priori error estimate

$$\|u - u_h\|_{V_h} \leq C(\Delta t^q + \Delta x^p) \left(\|\partial_t^{q+1} u\|_{L_2(Q)^J} + \|D^{p+1} u\|_{L_2(Q)^J} \right)$$

for Δt (maximal time step size), Δx (maximal spatial step size) and $1 \leq p := \min_K p_K$, $1 \leq q := \min_K q_K$.

The space-time approach avoids a CFL-stability condition but will lead to a huge linear system of equations that has to be solved. Thus we will try to reduce the number of unknowns and develop fast solution techniques. The resulting method has to run efficiently on a parallel computer.

Duality based goal-oriented error estimation. [3, Sect. 5] We assume that our computational goal can be achieved by minimising the error $e := u - u_h$ with respect to a given error functional $\mathcal{E} : V \rightarrow \mathbb{R}$. Then we can use the *dual problem*

$$(w, L^* u^*)_{L_2(Q)^J} = \mathcal{E}'[u](w) \quad \text{for all } w \in W$$

defining the dual solution $u^* \in V^*$ to get the error representation

$$\mathcal{E}(u) - \mathcal{E}(u_h) = -(Lu_h - f, u^* - u_h^*)_{L_2(Q)^J} + O(\|e\|_{L_2(Q)^J}^2)$$

with the discrete dual solution u_h^* [1]. From this the error can be estimated as

$$\begin{aligned} |\mathcal{E}(u) - \mathcal{E}(u_h)| &= |(Lu_h - f, u^* - u_h^*)_{L_2(Q)^J}| + O(\|e\|_{L_2(Q)^J}^2) \\ &\leq \sum_{R \in \mathcal{R}} \eta_R + O(\|e\|_{L_2(Q)^J}^2) \end{aligned}$$

with local residuals η_R depending on u_h and $u^* - u_h^*$. The unknown exact dual solution u^* is approximated from the computed solution u_h^* via a polynomial recovery u_r^* of higher polynomial order in space and time.

In the adaptive algorithm, the local quantities η_R are evaluated and a cell R is marked if $\eta_R \geq \theta \eta_{\max}$ for some $\theta \in (0, 1)$. On marked cells the polynomial degree in space and time is increased by one.

Space-time multilevel preconditioner. [3, Sect. 6] The system of equations is solved with GMRES and a multilevel preconditioner. The space-time hierarchy is defined to first coarsen in space up to the macro level and then to coarse in time. As a smoother in time we use the block-Jacobi method, in space we use the block Gauss–Seidel method, and on the coarse grid the (still large) system is solved by a parallel direct solver.

The method shows a convergence rate that depends on the CFL number $\Delta t/\Delta x$.

Numerical Tests for space-time adaptivity. The method has been tested on two examples [3, Sect. 7].

The first one is the linear transport equation $\partial_t u + \nabla \cdot (qu) = 0$ on $Q = [-10, 10]^2 \times [0, 1]$ for given $q(x) = 2\pi(-x_2, x_1)$ and compactly supported u_0 ("Rotating cone"). The error functional is given as $\mathcal{E}(v) = 1/2 (v, v)_{L_2(Q)}$. The adaptive method saves 90% of the unknowns compared to a uniform mesh.

The second example is a transverse electromagnetic wave in \mathbb{R}^2 in 3 components (H_1, H_2, E_3) (E electric, H magnetic field) that passes a double slit and interferes. The error functional is given as $\mathcal{E}(v) = 1/2 (v, v)_{L_2(S)^3}$, where $S \subset Q$ is a local space-time domain at the screen near the first minimum of the interference pattern. The adaptive method saves about 70% of the unknowns compared to a uniform mesh.

Both examples have been computed on a parallel machine with 256 or 1024 processors.

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A two-energies principle for the biharmonic equation and an a posteriori error bound for a discontinuous Galerkin method

DIETRICH BRAESS

(joint work with Astrid Pechstein, Joachim Schöberl)

There are many methods for estimating the error of a finite element solution a posteriori. We will use the two-energies principle, since it provides reliable error bounds without generic constants. It is also found under the names the 'hypercircle method by Prager and Synge', 'equilibrated error estimates', and 'error computation by local Neuman problems'. The error bound is usually computed in a postprocessing. The way of the computation depends on the considered elliptic differential equation and also on the finite element discretization.

In this framework we consider the biharmonic equation as a system of two equations of second order

$$(1) \quad \begin{aligned} \nabla^2 u &= \sigma && \text{in } \Omega, \\ \operatorname{div} \operatorname{div} \sigma &= f && \text{in } \Omega, \quad u = \frac{\partial u}{\partial n} = 0 \quad \text{on } \partial\Omega, \end{aligned}$$

The investigation of the two-energies principle is here new, while the application to differential equations of second order is now well known.

The solution of (1) can be characterized by a minimum problem

$$\int_{\Omega} \left[\frac{1}{2} \nabla^2 v : \nabla^2 v - f v \right] dx \longrightarrow \min_{v \in H_0^2(\Omega)} !$$

or by a maximum problem

$$-\frac{1}{2} \int_{\Omega} \tau : \tau dx \longrightarrow \max_{\substack{\tau \in H(\text{div}^2, \Omega) \\ \text{div div } \tau = f}} !$$

As indicated the maximum problem is subject to the equilibration condition (2). It is understood in the distributional sense

$$(2) \quad \langle \text{div div } \tau, w \rangle := \langle f, w \rangle, \quad w \in H_0^2(\Omega);$$

Here $\langle \cdot, \cdot \rangle$ is the $H^{-2}(\Omega) \times H_0^2(\Omega)$ product. It will be given explicitly for the double divergence operator and the finite elements of the Hellan–Herrmann–Johnson (HHJ) method in (6).

There is no duality gap between the minimum problem and the maximum problem above. The result is the following theorem.

The two-energies principle for the biharmonic equation.

Let $v \in H_0^2(\Omega)$ and $\tau \in L_2(\Omega)_{sym}^{2 \times 2}$ be equilibrated, i.e., (2) holds. If u is the solution of the biharmonic equation, then

$$(3) \quad \int_{\Omega} (\nabla^2(u - v))^2 dx + \int_{\Omega} (\nabla^2 u - \tau)^2 dx = \int_{\Omega} (\nabla^2 v - \tau)^2 dx.$$

Given an approximate solution v , the first term on the left-hand side of (3) provides an a posteriori error bound without generic constant for the error $v - u$ when an equilibrated tensor τ has been constructed and the right-hand side is known by assumption. As already mentioned, a postprocessing for this purpose is individually designed for each differential equation and each discretization.

Now, nonconforming or mixed methods are preferred for the FE solution of the biharmonic equation on a triangulation \mathcal{T}_h of Ω , since H^2 -conforming elements lead to involved implementations. Let $k \geq 2$. In particular discontinuous Galerkin methods with a space of piecewise polynomials,

$$V_h := \{v_h \in C^0(\Omega) \mid v_h|_T \in P_k(T), T \in \mathcal{T}_h(\Omega)\}.$$

are now popular [2]. The fact $V_h \not\subset H^2(\Omega)$ is compensated by an internal penalty (IP). The C^0 IPDG method penalizes the jumps of the derivatives on edges and adds terms to the variational form in order to keep the consistency,

$$\begin{aligned} A_h(u_h, v_h) := & \sum_{T \in \mathcal{T}_h(\Omega)} \int_T \nabla^2 u_h : \nabla^2 v_h dx + \sum_E \int_E \frac{\alpha}{h_E} [\partial_n u_h] [\partial_n v_h] ds \\ & - \sum_E \int_E \left([\partial_n u_h] \{ \nabla^2 v_{h,nn} \} + \{ \nabla^2 u_{h,nn} \} [\partial_n v_h] \right) ds. \end{aligned}$$

The penalty parameter α has to be sufficiently large. The weak finite element equations read

$$(4) \quad A_h(u_h, v_h) = (f, v_h)_{(0,\Omega)} \quad \forall v_h \in V_h.$$

In the framework of DG methods, the degrees of freedom of the C^0 polynomials in V_h are more involved than those for completely discontinuous ones; see [1, 4].

Next, we choose the spaces from the mixed method of Hellan–Herrmann–Johnson for the construction of the equilibrated tensors; see [3],

$$M_h := \{ \tau_h \in [L_2(\Omega)]_{sym}^{2 \times 2} \mid \tau_h|_T \in [P^{k-1}(T)]_{sym}^{2 \times 2}, T \in \mathcal{T}_h(\Omega), \\ \tau_{nn} \text{ is continuous at interelement boundaries} \}.$$

The spaces are not $H(\text{div div})$ conforming, but it is no drawback for the double divergence operator in distributional form.

The postprocessing for the construction of an equilibrated flux σ_h^{eq} is done by solving on each triangle T and its boundary ∂T an interpolation problem that is well defined due to [3]. The normal-normal components of the tensors play an important role for the interpolation

$$\sigma_{h,nn}^{eq} = -(\{\nabla^2 u_{h,nn}\} + \frac{\alpha}{h} [\partial_n u_h]) \in P^{k-1}(E), E \subset \partial T, \\ \int_T \sigma_h^{eq} : q \, dx = \int_T \nabla^2 u_h : q \, dx + \sum_{E \subset \partial T} \int_E \frac{1}{2} [\partial_n u_h] q_{nn} \, ds \\ \forall q \in [P^{k-2}(T)]_{sym}^{2 \times 2}.$$

By combining the variational equality (4) and the interpolation conditions above we obtain

$$(5) \quad \langle \text{div div } \sigma_h^{eq}, v_h \rangle = (f, v_h)_{0,\Omega} \quad \forall v_h \in V_h$$

Now we are close to our aim. We need the equation (5) not only for all test functions in V_h but also for all test functions in $H^2(\Omega)$. Such a small deviation from the aim is usually analyzed under the name *data oscillation*. We get the a posteriori estimation for a right hand side f_h that is an approximation of f . A formula for f_h is obtained from the representation of the operator $\text{div div} : M_h \rightarrow V_h^*$ is obtained by multiple partial integration,

$$(6) \quad \langle \text{div div } \sigma_h^{eq}, v \rangle = \sum_{T \in \mathcal{T}_h} \int_T \underbrace{\text{div div } \sigma_h^{eq}}_{\in P^{k-3}(T)} v \, dx \\ + \sum_E \int_E \underbrace{[-\partial_t \sigma_{h,nt}^{eq} - (\text{div } \sigma_h^{eq}) \cdot n_E]}_{\in P^{k-2}(E)} v \, ds \\ + \underbrace{\sum_V \sum_{E \supset V} \delta(E, V) [\sigma_{h,nt}^{eq}(V)]}_{\in \mathbb{R}} v(V).$$

The solution of the biharmonic equation for the right-hand side f_h differs from the correct one by a term of order $O(h^2)$ or higher. This deviation is consistent with the results for other methods of estimating a posteriori error estimates. Only a difference is worth to be noted. Here f_h is not an L_2 projection of f .

The analysis of the a posteriori error bounds for the discontinuous Galerkin method is very close to that for the discretization by the mixed method of Herrmann–Hellan–Johnson. The solution of the finite element method is already equilibrated. In particular the equilibrated tensors are obtained by local constructions on each element separately. On the other hand, the postprocessing is performed usually on larger patches of the triangulation in the case of conforming elements.

Thus the discontinuous Galerkin methods turn out to be as favorable as mixed methods. Roughly speaking the DG methods are located between the primal and the mixed methods. This is an advantage that makes the methods so popular.

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Adaptive finite element methods for Stokes eigenvalue problems

JOSCHA GEDICKE

(joint work with Arbaz Khan)

Over the last decade, the *a posteriori* error analysis of eigenvalue problems using finite element approximations has been well developed. However, most results are for the Laplace eigenvalue problem and only a few papers consider the *a posteriori* error analysis for the Stokes eigenvalue problem. Lovadina et al. [1] present the *a posteriori* error analysis based on residual error estimators for the finite element discretization of the Stokes eigenvalue problem. In [2], Liu et al. propose the finite element approximation of Stokes eigenvalue problems based on a projection method, and derive some superconvergence results and related recovery type *a posteriori* error estimators. *A posteriori* error estimates for stabilized low-order mixed finite elements for the Stokes eigenvalue problem are presented by Armentano et al. [3]. A new adaptive mixed finite element method based on residual type *a posteriori* error estimates for the Stokes eigenvalue problem is proposed by Han et al. [4].

It is the aim of this talk to present the *a posteriori* error analysis for the Stokes eigenvalue problem based on two additional finite element discretizations which enable higher order approximations of Stokes eigenvalues.

In the first part we study the Arnold-Winther mixed finite element formulation for the two-dimensional Stokes eigenvalue problem using the stress-velocity formulation. Arnold and Winther introduced a strongly symmetric mixed finite element (MFEM) for linear elasticity in [5] and proved it to be stable for any material parameters. Hence, the Arnold-Winther MFEM is also stable for the Stokes problem as a limit case of linear elasticity. We present *a priori* error estimates for eigenvalues and eigenfunctions for the Arnold-Winther MFEM discretization of the Stokes eigenvalue problem. To improve the approximation for eigenvalues and eigenfunctions, we use local postprocessing. For smooth data we prove higher order convergence of the postprocessed eigenvalues. With the help of the higher order local postprocessing, we develop a reliable *a posteriori* error estimator. We discuss several numerical examples to validate the theoretical higher order convergence of the postprocessing and the reliability and empirical efficiency of the derived *a posteriori* error estimator.

In the second part we present the *a posteriori* error analysis of H^{div} -conforming discontinuous Galerkin finite elements for Stokes eigenvalue problems based on Cockburn et al. [6, 7]. For the velocity-pressure formulation we present *a priori* error estimates for eigenvalues and eigenfunctions. We develop the *a posteriori* error analysis of H^{div} -conforming discontinuous Galerkin finite elements for the Stokes eigenvalue problem and prove upper and local lower bounds for the velocity-pressure error which is measured in terms of a mesh-dependent energy norm. The reliability and efficiency of the proposed *a posteriori* error estimator is verified by numerical examples which include higher order discretizations with up to third order polynomials.

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A posteriori error estimators for hybrid finite element methods

JAEUN KU

(joint work with Young Ju Lee and Dongwoo Sheen)

We present a new numerical method for second order elliptic partial differential equations in [KLS]. The method is a two-step method based on the hybridization of mesh sizes in the traditional mixed finite element method. On a coarse mesh, a crude approximation u_H^G for the primary variable u is obtained by a standard Galerkin method, whose computational cost is very low. Then, on a fine mesh, an $H(\text{div})$ projection of the dual variable σ is sought as an accurate approximation for the flux variable with the crude approximation u_H^G as a part of problem, i.e., find $\sigma_h \in V_h \subset H(\text{div} : \Omega)$ such that

$$(\nabla \cdot \sigma_h, \nabla \cdot \tau_h) + \delta(\sigma_h, \tau_h) = (f + \delta u_H^G, \tau_h), \text{ for all } \tau_h \in V_h.$$

We show that the finer mesh size h can be taken as the square of the coarse mesh size H , or a higher order power with a proper choice of parameter δ . This means that the computational cost for the coarse-grid solution is negligible compared to that for the fine-grid solution. In fact, numerical experiments show an advantage of using our strategy compared to the mixed finite element method.

Our method does not rely on the framework of traditional mixed formulations, the choice of pair of finite element spaces is, therefore, free from the requirement of the inf-sup stability condition. More precisely, our method is formulated in a fully decoupled manner, still achieving an optimal error convergence order. This leads to a computational strategy much easier and wider to implement than the mixed finite element method. Additionally, the independently posed solution strategy allows to use different meshes as well as different discretization schemes in the calculation of the primary and flux variables.

The main motivation of our new method is obtaining an accurate and efficient approximation for the flux variables. To estimate and control the error of the flux variables, we present a posteriori error estimates that apply to Raviart-Thomas and Brezzi-Douglas-Marini elements. The estimator has the same terms for the a posteriori error estimators for the mixed Galerkin method presented in [A], and additional higher order terms. We establish efficiency and reliability bounds for the estimator. The convergence of adaptive procedure based on the error estimator could be obtained using the technical tools developed in [CH]. This is still an open problem.

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Recovery-based error estimation for stress-based mixed finite element methods in elasticity and plasticity

GERHARD STARKE

The stress-based mixed finite element formulation relies on suitable subspaces $\Sigma_h \subset H(\text{div}, \Omega)^d$, $\mathbf{V}_h \subset L^2(\Omega)^d$ and $\mathbf{R}_h \subset L^2(\Omega)^{d \times d, \text{as}}$ and consists in finding $(\sigma_h, \mathbf{u}_h, \rho_h) \in \Sigma_h \times \mathbf{V}_h \times \mathbf{R}_h$ such that

$$\begin{aligned} (\mathcal{A}\sigma_h, \tau_h)_{L^2(\Omega)} + (\mathbf{u}_h, \text{div } \tau_h)_{L^2(\Omega)} + (\rho_h, \text{as } \tau_h)_{L^2(\Omega)} &= 0, \\ (\text{div } \sigma_h + \mathbf{f}, \mathbf{v}_h)_{L^2(\Omega)} &= 0, \\ (\text{as } \sigma_h, \vartheta_h)_{L^2(\Omega)} &= 0 \end{aligned}$$

holds for all $(\tau_h, \mathbf{v}_h, \vartheta_h) \in \Sigma_h \times \mathbf{V}_h \times \mathbf{R}_h$. Here, $L^2(\Omega)^{d \times d, \text{as}}$ denotes the space of antisymmetric matrix-valued functions, as stands for the antisymmetric part and \mathcal{A} abbreviates the stress-strain mapping

$$\mathcal{A}\tau = \frac{1}{2\mu} \left(\tau - \frac{\lambda}{3\lambda + 2\mu} (\text{tr } \tau) \mathbf{I} \right)$$

from linear (small-strain) elasticity with Lamé parameters λ and μ . The displacements \mathbf{u}_h and the rotations ρ_h take the role of Lagrange multipliers associated with the constraints consisting of momentum balance and stress symmetry, respectively. A possible combination of finite element spaces satisfying the inf-sup condition is given by using next-to-lowest order Raviart-Thomas elements (RT_1) for Σ_h in connection with piecewise linears for \mathbf{V}_h and piecewise linear continuous functions for \mathbf{R}_h , see [1].

For this formulation, an a posteriori error estimator based on reconstructed H^1 -conforming displacements is investigated. Due to the relation

$$-(\mathbf{u}_h, \text{div } \tau_h) = (\mathcal{A}\sigma_h, \tau_h) + (\rho_h, \text{as } \tau_h) = (\mathcal{A}\sigma_h + \rho_h, \tau_h),$$

the discontinuous piecewise quadratic approximation $\mathbf{g}_h = \mathcal{A}\sigma_h + \rho_h$ to $\nabla \mathbf{u}$ may be used as a starting point for the following gradient reconstruction algorithm (cf. [3], [6], and also the earlier work [5]):

Step 1. For each $T \in \mathcal{T}_h$, determine $\mathbf{u}_h^\circ|_T \in P_2(T)^d$ such that

$$\begin{aligned} (\nabla \mathbf{u}_h^\circ, \nabla \mathbf{v}_h)_{L^2(T)} &= (\mathbf{g}_h, \nabla \mathbf{v}_h)_{L^2(T)} \text{ for all } \mathbf{v}_h \in P_2(T)^d, \\ (\mathbf{u}_h^\circ, \mathbf{e}_i)_{L^2(T)} &= (\mathbf{u}_h, \mathbf{e}_i)_{L^2(T)} \text{ for } 1 \leq i \leq d. \end{aligned}$$

Step 2. Construct $\mathbf{u}_h^R \in P_2(\mathcal{T}_h)^d \subset H^1(\Omega)^d$ by averaging:

$$\mathbf{u}_h^R(\mathbf{x}) = \frac{1}{\#\{T : \mathbf{x} \in T\}} \left(\sum_{T: \mathbf{x} \in T} \mathbf{u}_h^\circ|_T(\mathbf{x}) \right).$$

That the associated least-squares functional

$$\eta := \|\mathcal{A}\sigma_h - \varepsilon(\mathbf{u}_h^R)\|_{L^2(\Omega)} = \left(\sum_{T \in \mathcal{T}_h} \|\mathcal{A}\sigma_h - \varepsilon(\mathbf{u}_h^R)\|_{L^2(T)}^2 \right)^{1/2} =: \left(\sum_{T \in \mathcal{T}_h} \eta_T^2 \right)^{1/2}$$

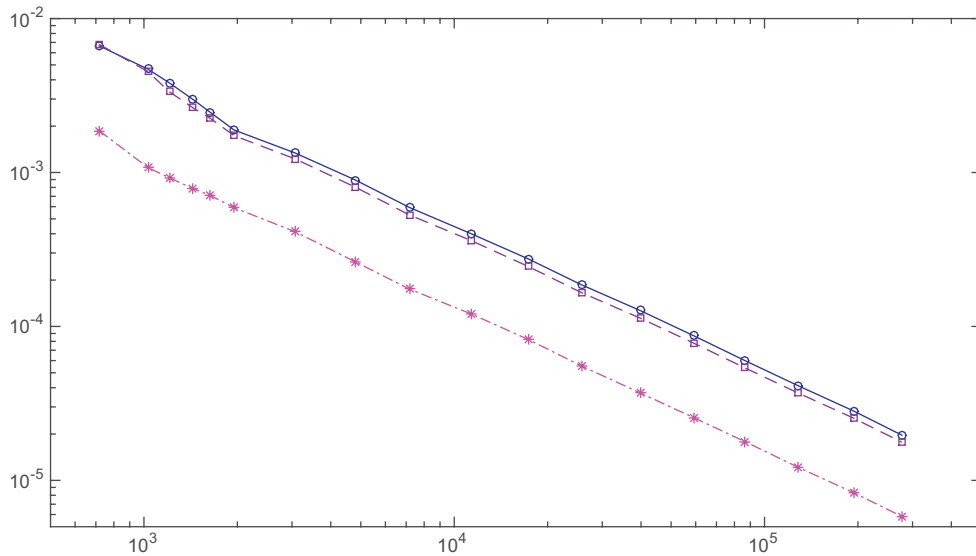


FIGURE 1. Convergence behavior (estimator η vs. degrees of freedom)

constitutes an a posteriori error estimator, uniformly in the incompressible limit as $\lambda \rightarrow \infty$, follows from [2]. The performance of the error estimator was tested numerically in an adaptive framework using the following equilibration refinement strategy: Mark a subset $\widehat{\mathcal{T}}_h \subset \mathcal{T}_h$ for refinement such that

$$\left(\sum_{T \in \widehat{\mathcal{T}}_h} \eta_T^2 \right)^{1/2} \geq \theta \left(\sum_{T \in \mathcal{T}_h} \eta_T^2 \right)^{1/2}$$

(with $\theta = 0.8$ in our computations). For the standard Cook's membrane problem with corners $(0, 0)$, $(0.48, 0.44)$, $(0.48, 0.6)$ and $(0, 0.44)$ and boundary conditions $\mathbf{u} = \mathbf{0}$ at the left, $\boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{0}$ at the top and bottom, and $\boldsymbol{\sigma} \cdot \mathbf{n} = (0, 1)$ at the right boundary component, the convergence behavior is shown in Figure 1.

During the course of 17 adaptive refinement steps, the solid curve shows the convergence behavior using \mathbf{u}_h^R from the above averaging algorithm. The dashed curve slightly below shows the results obtained if \mathbf{u}_h^R is replaced by \mathbf{u}_h^* minimizing the distance $\nabla \mathbf{u}_h^*$ to \mathbf{g}_h with respect to the $L^2(\Omega)$ norm (which involves a global variational problem to be solved). The dash-dotted line below shows the behavior of the antisymmetric part as $\boldsymbol{\sigma}_h$.

The generalization to small-strain elastoplasticity of von Mises type is done by introducing a third Lagrange multiplier associated with the yield criterion. This Lagrange multiplier space is represented again by piecewise linear continuous finite elements and involve an additional sign condition. The a posteriori error estimation can again be carried out using the corresponding least-squares functional based on the analysis in [4].

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Mesh refinement for large, complex, realistic problems

WOLFGANG BANGERTH

Introduction. The techniques for estimating the error in finite element computations date back to work by Babuška et al. in the late 1970s and early 1980s (see, for example, [1, 9, 8]). At the time, however, the software technology did not exist to use error estimators as refinement criteria for adaptive mesh refinement, and these papers initially had little practical impact. This all changed with the advent of widely usable software packages in the mid-1990s and early 2000s that encapsulated the complex data structures and algorithms necessary for adaptive mesh refinement, and made them generically available for a broad class of finite element solvers. This also coincided with the publication of the influential survey of Verfürth on error estimators and adaptive meshing techniques in 1996 [11], and books such as [7] on computational meshes. Together, these books popularized the methods necessary for *practical* use of error estimators and mesh adaptation.

Adaptive mesh refinement techniques are unquestioningly more efficient than other methods in yielding highly accurate solutions of partial differential equations. Conversely, they can yield the same accuracy with a fraction of the computational cost. All major finite element packages, as well as many commercial codes today offer and use adaptive mesh refinement. They are available for single machine computations but have also been shown to scale to the largest available parallel machines [3, 10, 2, 6].

On the other hand, the majority of adaptive mesh refinement applications today do not seem to be driven by (“a posteriori”) error *estimators* that rigorously bound the error by expressions that only involve the numerical solution computed on a previous mesh. Rather, most practical applications seem to drive mesh refinement through error *indicators* that suggest on which cells the error may be large. These indicators are typically chosen heuristically, using analogies to simpler equations for which they may have been derived as rigorous estimators, or simply because they estimate the *interpolation error*, even though the relationship between the interpolation error and the finite element projection error may not be clear.

A common example for such error indicators is the widely used “Kelly indicator” [9, 8] that is implemented in many finite element software packages. Originally derived as an error estimator for the Laplace equation, it is widely employed as a refinement criterion for any number of other equations that have little in common with the elliptic Laplace equation with its smooth solutions. The success of the method is typically attributed to the fact that it approximates the size of the second derivatives of the solution, which is both an estimate of the finite element error of the Laplace equation, as well as the interpolation error for the solution of any, generic partial differential equation. It therefore often leads to meshes that may not be optimal for a given equation, but that are still very good and vastly better than global mesh refinement or refinement “by hand”.

Given the fact that rigorous error estimators are not widely used in actual practice, it is interesting to revisit what the obstacles are that prevent us from using them for more applications. I will summarize my thoughts in the following six subsections. I will prefix this discussion by stating that any method one can think of will have to be able to solve *realistic problems*, i.e., problems that may be coupled, nonlinear, time dependent, and that possibly require thousands of processors to solve. These requirements separate such problems from *model problems* such as the Laplace, Stokes, or advection equation for which methods based on rigorous error estimates are widely available, but that are often only simplified building blocks of models used in practice.

Obstacle 1: Realistic problems are coupled and nonlinear. The vast majority of published estimators are for relatively simple, linear model problems and at one point or other rely on a stability estimate. However, practical applications are typically nonlinear and may couple different effects – such as thermal diffusion and advection coupled with flow problems where the viscosity depends on temperature. For this kind of problem, rigorous estimates of stability – or of anything else, in fact – are almost never available. These problems may not inherently lack stability or other necessary ingredients for error estimators, but we lack the mathematical technology to *prove* these properties. Consequently, for most problems of practical interest, no rigorously derived error estimators are available.

Duality-based estimators (see, e.g., [5, 4]) work around this by *computing* stability and other properties. They can also incorporate a goal functional with respect to which we may want to estimate the error. For many problems, including complex nonlinear problems, duality-based error estimators have been shown to be very efficient, but they yield other difficulties as discussed in the following.

Obstacle 2: Duality-based error estimates cannot be used for time dependent problems. Duality-based error estimators require the solution of an adjoint problem linearized around the forward solution. For time dependent problems, this means storing the forward solution at each time step, solving a dual problem backward in time and storing the solution, and then computing estimators for all time steps. Although there are some approaches to make this workflow

more tractable (e.g., checkpointing), the amount of data handling necessary is often considered prohibitive, and duality-based methods have not found widespread acceptance for time dependent problems.

Obstacle 3: Duality-based error estimates do not scale to large parallel problems. Duality-based methods can not find the mesh for one time step by adapting an already fine mesh from the previous time step. Rather, they need to solve forward and backward problems on a sequence of relatively coarse meshes. This cannot be done efficiently on large parallel meshes because of the limits of strong scalability. Efficient implementations would therefore have to use successively larger numbers of processors, but adjusting the number of processors is not an option with current management practices of shared parallel machines.

Obstacle 4: In complex applications, the choice of goal functional or error norm is typically not clear. Traditional error estimators use a natural norm of the problem to estimate the error in. Goal-oriented approaches replace this by a single, scalar functional of the solution. However, in many practical applications in which one wants to *discover behavior of solutions*, it is not at all clear what scalar measure one should try to minimize the error in.

Obstacle 5: Residual-based indicators are difficult for coupled problems. A common approach is therefore to refine simply based on a norm of the residual, multiplied by some power of the mesh size. However, coupled problems have multiple residuals, each with their own and separate physical units. It is therefore not typically clear how to combine them into a single measure for each cell that would suggest the size of the error.

Obstacle 6: What do we want to approximate anyway? In many applications, it is not clear whether minimizing the error in the *solution* is useful at all. Rather than solution variables (e.g., velocity, pressure, and temperature in thermally driven flow), one may be interested in nonlinear combinations (e.g., the strain-rate and temperature dependent viscosity) or in non-local and ill-defined quantities such as “how far do continents typically drift apart over 100 million years”. For these quantities, the relationship to the error in the solution is often difficult to assess, and minimizing an error norm may not be a useful strategy.

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Adaptivity in High-Order Finite Element ALE Simulations

TZANIO KOLEV

(joint work with R. Anderson, Z. Cai, J. Cervený, V. Dobrev, C. He, R. Rieben
and M. Stowell)

¹ The Arbitrary Lagrangian-Eulerian (ALE) framework forms the basis of many large-scale multi-physics codes, and in particular those centered around radiation diffusion [2] and shock hydrodynamics. We are developing general high-order finite element discretization framework that aims to improve the quality of current ALE simulations, while also improving their performance on modern data-centric computing architectures. We use the de Rham complex to guide the discretization of different physics components. In particular, H^1 finite elements are used to discretize kinematic quantities (e.g. velocity, position), $H(\text{curl})$ finite elements are employed for the electric field in magneto-hydrodynamics (MHD) models, $H(\text{div})$ finite elements are used for the flux in radiation diffusion, and discontinuous L^2 finite elements represent thermodynamic quantities (e.g. internal energy).

Adaptive mesh refinement (AMR) as oppose to uniform mesh refinement is an important tool editing the mesh aiming to achieve the desired accuracy at the minimal possible cost. One of the key components in AMR is the a posteriori error estimation. A competent error estimation often features generality, accuracy and cost-effectivity. Error estimation for linear conforming finite element on conforming triangular meshes has gained the vast majority of research interest in the last four decades [4, 7]. Nevertheless, there has limited work on the error estimation of high order finite element methods or of the nonconforming quadrilateral mesh with hanging nodes[3, 6]. In contrast, nonconforming quadrilateral meshes are broadly accepted and applied in the engineering and industry practice.

To address adaptivity in these settings, we have developed general capability by applying a ZZ-like (anisotropic) recovery based error estimation[8, 7] that support adaptive mesh refinement on triangular, quadrilateral and hexahedral curvilinear

¹Work Performed under the auspices of the U.S. Department of Energy under Contract DE-AC52-07NA27344 (LLNL-ABS-705907).

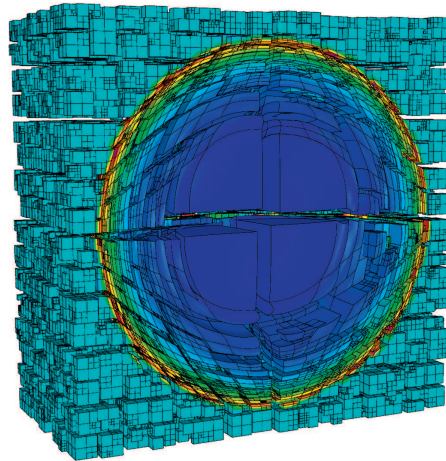


FIGURE 1. Radial shock propagation in high-order unstructured non-conforming mesh. Note the lack of mesh imprinting and shock reflections due to hanging nodes.

meshes, at arbitrarily high order, for any finite element space, in both two and three dimensions. We can as well handle complex 3D anisotropic refinements, unlimited refinement levels of adjacent elements, and MPI parallelism with load balancing [1]. In this talk we present the high-order AMR algorithms and demonstrate their performance on model compressible hydrodynamics and computational electromagnetic problems, see Fig1.

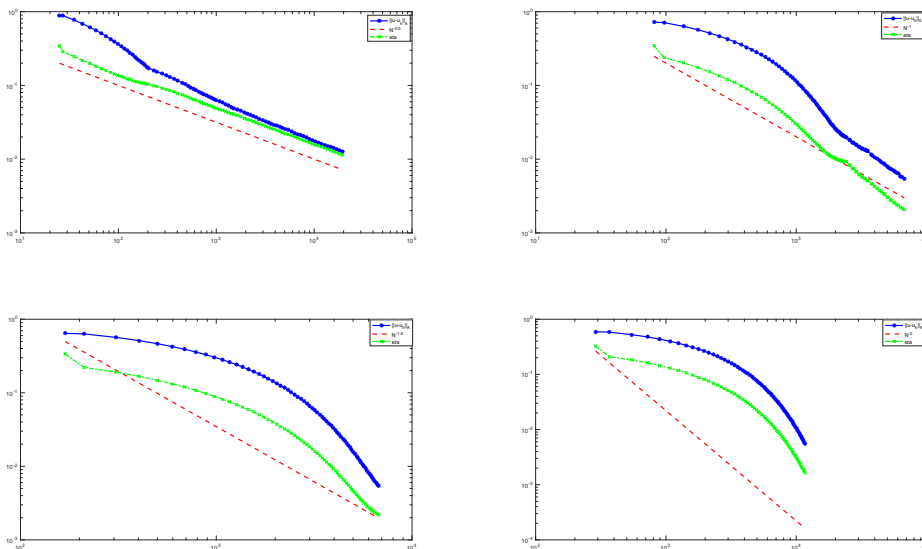


FIGURE 2. Initial results with a local flux-recovery error estimator for H1 problems, orders 1–4.

One possible drawback of the ZZ-like (anisotropic) approach is its tendency to solve global projection problem and hence cost expensive. Our ongoing efforts on adaptivity focus on designing and developing a local ZZ-like error estimation that preserves the generality and accuracy and at the same time achieves the highly cost-effectivity[5]. This method has shown promising numerical results for arbitrary high order H^1 elements on any mesh, see Fig2. We are exploring its extension to the rest of de Rham sequence.

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Optimality of Adaptive Methods

LARS DIENING

In this talk we show how different marking strategies result in different optimality concepts. Our model case is the Poisson equation and its variational formulation. We will see that the Dörfler strategy is related to rate optimality and the maximum strategy is related to energy optimality.

To keep the setup as simple as possible, we consider the standard Poisson equation $-\Delta u = f$ on a polyhedral domain $\Omega \subset \mathbb{R}^2$ combined with zero boundary values for u and $f \in L^2$. Then the unique solution $u \in W_0^{1,2}(\Omega)$ is also the unique minimizer of the Dirichlet energy $\mathcal{J} : W_0^{1,2}(\Omega) \rightarrow \mathbb{R}$ given by

$$\mathcal{J}(v) := \int_{\Omega} \frac{1}{2} |\nabla v|^2 dx - \int_{\Omega} v f dx.$$

Starting from a macro triangulation \mathcal{T}_0 we consider triangulations \mathcal{T} generated by newest vertex bisection. By $V(\mathcal{T})$ we denote the subspace of $W_0^{1,2}(\Omega)$ of piecewise linear functions.

We assume that our sequence of triangulations \mathcal{T}_k is generated by the usual AFEM loop (Solve-Estimate-Mark-Refine). By $u_{\mathcal{T}_k} \in V(\mathcal{T}_k)$ we denote the corresponding discrete solution, which is just the minimizer of \mathcal{J} on $V(\mathcal{T}_k)$. Since our

triangulations and our spaces $V(\mathcal{T}_k)$ are nested, the energies $\mathcal{J}(u_{\mathcal{T}_k})$ decrease. To steer the refinement we need suitable local error estimators $\mathcal{E}_{\mathcal{T}}^2$ depending on $u_{\mathcal{T}_k}$.

So far two marking strategies are known to provide optimal convergence of the AFEM algorithm in terms of accuracy versus degrees of freedom:

- (a) Dörfler strategy: Mark the (almost) smallest set that contains at least a θ_* -fraction of the total error estimator, i.e. $\mathcal{E}_{\mathcal{T}}^2(\text{marked}) \geq \theta_* \mathcal{E}_{\mathcal{T}}^2(\Omega)$.
- (b) Maximum strategy: Refine where the error estimator is comparable to the maximal one, i.e. mark those edges S with $\mathcal{E}_{\mathcal{T}}^2(S) \geq \frac{1}{2} \max \mathcal{E}_{\mathcal{T}}^2$.

Numerous article have appeared on the optimality of the Dörfler strategy, which are based on the seminal articles [1, 4]. See [2] for an axiomatic summary. The optimality of the maximum strategy goes back to [3]. Although both marking strategies provide optimality, the underlying optimality concepts differ which is the focus of this talk.

To gain more insight we have to look closer at the variational structure. Our algorithm is clearly driven by an energy minimization. For a refinement \mathcal{T}_* of \mathcal{T} we have $\frac{1}{2} \|\nabla u_{\mathcal{T}} - \nabla u_{\mathcal{T}_*}\|_2^2 = \mathcal{J}(u_{\mathcal{T}}) - \mathcal{J}(u_{\mathcal{T}_*})$. Hence, we can replace the usual gradient error by the simpler concept of energy differences. It is well known that the error estimators do not control the error but the total error, which is the sum of the error plus data oscillations. By considering the relaxed energy $\mathcal{G}(\mathcal{T}) := \mathcal{J}(u_{\mathcal{T}}) + \text{osc}^2(\mathcal{T})$ as in [3] it is possible to pass to an equivalent minimization problem, which takes care of this oscillation problem. Overall, our relaxed energy and our estimators are linked by the following optimal estimate.

$$(1) \quad \|\nabla u_{\mathcal{T}} - \nabla u_{\mathcal{T}_*}\|_2^2 + \text{osc}^2(\text{refined}) \approx \mathcal{E}_{\mathcal{T}}^2(\text{refined}) \approx \mathcal{G}(\mathcal{T}) - \mathcal{G}(\mathcal{T}_*).$$

At this the oscillation and the estimators are only evaluated on the refined parts.

For both marking strategies the algorithm reduced in each step the energy $\mathcal{G}(\mathcal{T}_k)$ converging to the minimal energy $\mathcal{G}(\mathcal{T}_{\infty}) := \mathcal{J}(u)$. This is illustrated in the following pictures by the line from \mathcal{T}_0 to \mathcal{T}_{k+1} .

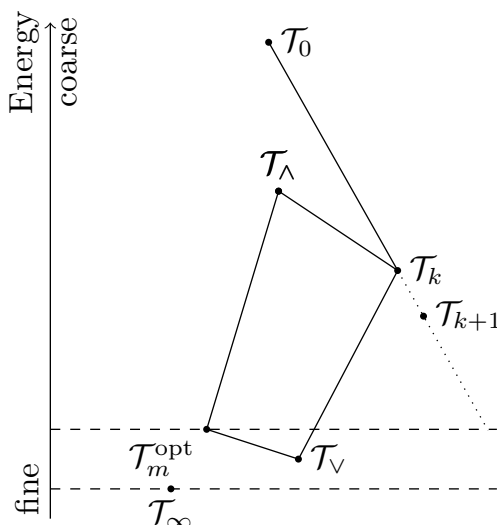


Figure D: Dörfler marking

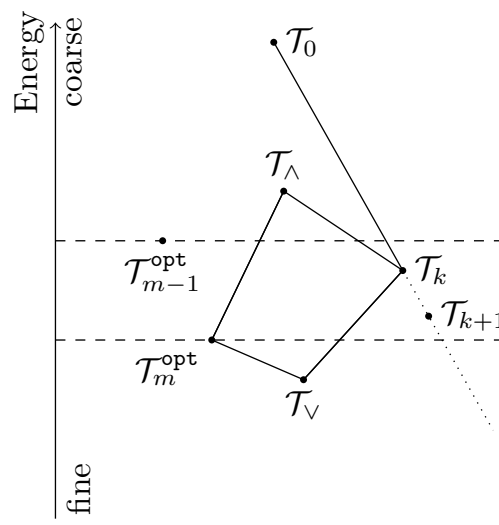


Figure M: Maximum strategy

The important point is how the optimality enters the picture. For this let $\mathcal{T}_m^{\text{opt}}$ denote the triangulation with m extra degrees of freedom (compared to \mathcal{T}_0) that has the smallest energy \mathcal{G} .

Let us consider the Dörfler strategy: The marking $\mathcal{E}_{\mathcal{T}}^2(\text{marked}) \geq \theta_* \mathcal{E}_{\mathcal{T}}^2(\Omega)$ and (1) imply a linear energy reduction, i.e. $\mathcal{G}(\mathcal{T}_{k+1}) - \mathcal{G}(\mathcal{T}_{\infty}) \leq \lambda(\mathcal{G}(\mathcal{T}_k) - \mathcal{G}(\mathcal{T}_{\infty}))$ with some $\lambda \in (0, 1)$. This allows essentially to reduce the complexity analysis of the sequence to the analysis of the step from \mathcal{T}_k to \mathcal{T}_{k+1} . Now, let us choose for k fixed the smallest triangulation $\mathcal{T}_m^{\text{opt}}$ such that $\mathcal{G}(\mathcal{T}_m^{\text{opt}}) - \mathcal{G}(\mathcal{T}_{\infty})$ is much smaller than $\mathcal{G}(\mathcal{T}_k) - \mathcal{G}(\mathcal{T}_{\infty})$. Then also $\mathcal{G}(\mathcal{T}_k) - \mathcal{G}(\mathcal{T}_v)$ is much smaller and hence $\mathcal{G}(\mathcal{T}_k) - \mathcal{G}(\mathcal{T}_v) \gtrsim \mathcal{G}(\mathcal{T}_k) - \mathcal{G}(\mathcal{T}_{\infty})$. Now the fundamental observation of [4] is that this implies (non-optimal) Dörfler marking due to (1). Since the Dörfler strategy chooses the smallest set for refinement, this is the access to optimality: we can estimate the complexity of the marked set in our algorithm from above by m , the additional complexity of $\mathcal{T}_m^{\text{opt}}$! This implies together with the linear energy reduction and mesh refinement estimates that for $s > 0$

$$(\#\mathcal{T}_k - \#\mathcal{T}_0)^s (\mathcal{G}(\mathcal{T}_k) - \mathcal{G}(\mathcal{T}_{\infty})) \leq c \sup_m (m^s (\mathcal{G}(\mathcal{T}_m^{\text{opt}}) - \mathcal{G}(\mathcal{T}_{\infty}))).$$

Depending on s the right-hand side determines (if it is finite) the best possible rate of degrees of freedom vs. accuracy. Therefore, Dörfler marking corresponds to rate optimality.

Now, let us consider the maximum strategy. In principle, it would be possible that only a single bisection is performed in each AFEM iteration. This situation turns out to be the critical one in the analysis. It is clear that a single bisection cannot reduce the energy by a fixed factor. Instead, let m denote the smallest number, such that $\mathcal{G}(\mathcal{T}_k)$ is still above the optimal energy $\mathcal{G}(\mathcal{T}_m^{\text{opt}})$, see Figure M. Then the crucial observation in [3] is that the single bisection reduces the energy by a fixed fraction of the energy gap $\mathcal{G}(\mathcal{T}_{m-1}^{\text{opt}}) - (\mathcal{T}_m^{\text{opt}})$. Hence, it only takes a finite number of bisection such that the energy of our algorithm falls below the next optimal energy level $\mathcal{G}(\mathcal{T}_m^{\text{opt}})$. Overall, the algorithm marches through the optimal energy levels. In particular, if $\#\mathcal{T}_k - \#\mathcal{T}_0 \geq cm$, then $\mathcal{G}(\mathcal{T}_k) \leq \mathcal{G}(\mathcal{T}_m^{\text{opt}})$. This is also called *energy optimality*. By equivalence of the energy differences with the total error, this implies *instance optimality* of the total error, i.e. if $\#\mathcal{T}_k - \#\mathcal{T}_0 \geq cm$, then $\|\nabla u_{\mathcal{T}_k} - \nabla u\|_2^2 + \text{osc}^2(\mathcal{T}_k) \leq c_2 \|\nabla u_{\mathcal{T}_m^{\text{opt}}} - \nabla u\|_2^2 + \text{osc}^2(\mathcal{T}_m^{\text{opt}})$.

The crucial observation of [3] itself is based on (1), mesh refinement properties, but also on an important extra property of our variational problem: the lower diamond estimate. The error indicator estimate (1) implies that the reduction of the energy when refining multiple (disjoint) areas is comparable to the sum of those reductions, if only one of those areas is refined. The lower diamond estimate states that the same is true for the coarsening of multiple (disjoint) areas. Note that the lower diamond estimate is not used in the analysis of the Dörfler strategy.

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The role of oscillation in a posteriori error analysis

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(joint work with Andreas Veeger)

A posteriori error estimators are a key tool for the quality assessment of finite element approximations as well as for the application of adaptive techniques. They aim at a precise quantification of the discretisation error in a computable manner. Unfortunately, all a posteriori estimators are equivalent to the error only up to some extra additive term – the so-called *oscillation* – which bounds the distance between non-discrete and discrete data. It can therefore be construed as an indicator for the estimator quality. In fact, oscillation can be significantly larger than the error which interferes with the objectives of a posteriori error analysis.

We shall first illustrate the shortcomings of the *classical* oscillation before presenting a new approach to a posteriori analysis which leads to an *error-dominated* oscillation thereby overcoming the shortcomings of the classical approach.

For the sake of a clear presentation, we restrict ourselves to the simplest case where $u \in H_0^1(\Omega)$ is the solution of Poisson’s problem

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

and the finite element approximation U is the Galerkin solution in the space $\mathbb{V}(\mathcal{M})$ of continuous and piecewise affine functions over some exact and shape regular simplicial partition \mathcal{M} of Ω .

1. SHORTCOMINGS OF THE CLASSICAL OSCILLATION

If $f \in L^2(\Omega)$, then e.g. the standard residual based estimator is given by

$$\mathcal{E}_R(U, f, \mathcal{M}) := \left(\sum_{K \in \mathcal{M}} h_K \|J(U)\|_{L^2(\partial K)}^2 + h_K^2 \|f\|_{L^2(K)}^2 \right)^{1/2}$$

and satisfies

$$\|u - U\|_{H_0^1(\Omega)} \lesssim \mathcal{E}_R(U, f, \mathcal{M}) \quad \text{and} \quad \mathcal{E}_R(U, f, \mathcal{M}) \lesssim \|u - U\|_{H_0^1(\Omega)} + \text{osc}_0(f, \mathcal{M})$$

with oscillation

$$\text{osc}_0(f, \mathcal{M})^2 := \sum_{K \in \mathcal{M}} h_K^2 \|f - P_{0, \mathcal{M}} f\|_{L^2(K)}^2 \quad \text{with} \quad P_{0, \mathcal{M}} f|_K := \frac{1}{|K|} \int_K f;$$

see e.g. [1, 3]. If $f \in H^1(\Omega)$ then

$$(1) \quad \text{osc}_0(f, \mathcal{M})^2 \lesssim \sum_{K \in \mathcal{M}} h_K^4 \|\nabla f\|_{L^2(K)}^2.$$

This observation is widely used to motivate that the oscillation is a negligible higher order perturbation of the estimator. However, on any fixed mesh \mathcal{M} the oscillation can be arbitrarily larger than the error. This is a consequence of the fact that $L^2(\Omega)$ is dense in $H^{-1}(\Omega)$ and that the L^2 -norm is strictly stronger than the H^{-1} norm, i.e., there exist $f \in L^2(\Omega)$, such that

$$\text{osc}_0(f, \mathcal{M})^2 = \sum_{K \in \mathcal{M}} h_K^2 \|f - P_{0, \mathcal{M}} f\|_{L^2(K)}^2 \gg \|f\|_{H^{-1}(\Omega)}^2 \geq \|u - U\|_{H_0^1(\Omega)}^2.$$

The use of the scaled L^2 -norm in the oscillation originates from its use in the element residual $h_K^2 \|f\|_{L^2(K)}$ and can be motivated by the request for the computability of the estimator, i.e., the evaluation of local H^{-1} -norms is reduced to the (approximative) evaluation of local integrals. However, Cohen, DeVore, and Nocketto observed in [2] that this is not the sole reason for possible overestimation. In fact, based on the generalised a posteriori bounds

$$(2) \quad \|u - U\|_{H_0^1(\Omega)}^2 \approx \sum_{z \in \mathcal{V}} \|\Delta U + f\|_{H^{-1}(\omega_z)}^2 \lesssim \sum_{z \in \mathcal{V}} \|\Delta U\|_{H^{-1}(\omega_z)}^2 + \|f\|_{H^{-1}(\omega_z)}^2$$

they proved that for certain right-hand sides f , the term $\sum_{z \in \mathcal{V}} \|f\|_{H^{-1}(\omega_z)}^2$ vanishes slightly slower than the error. Here \mathcal{V} denotes the vertices of \mathcal{M} and $\omega_z := \bigcup \{K \in \mathcal{M} : z \in K\}$. Note that the same phenomenon appears for e.g. $\text{osc}_{-1}(f, \mathcal{M})^2 := \sum_{z \in \mathcal{V}} \min_{f_z \in \mathbb{R}} \|f - f_z\|_{H^{-1}(\omega_z)}^2$. The reason for this effect is the splitting

$$\|\text{Res}(U)\|_{H^{-1}(\omega_z)} \leq \|\Delta U\|_{H^{-1}(\omega_z)} + \|f\|_{H^{-1}(\omega_z)}$$

of the residual $\text{Res}(U) = \Delta U + f$. Note that ΔU is discrete and thus is equivalent to the jump residual whereas $\|f\|_{H^{-1}(\omega_z)}$ is not computable in general. The splitting, however, may cause loss of cancellations: Assume that $f = -\Delta V \in H^{-1}(\Omega)$ for some $0 \neq V \in \mathbb{V}(\mathcal{M})$, then $U = V$ and thus $\text{Res}(U) = 0$ in contrast to

$$\sum_{z \in \mathcal{V}} \|\Delta U\|_{H^{-1}(\omega_z)}^2 = \sum_{z \in \mathcal{V}} \|f\|_{H^{-1}(\omega_z)}^2 \neq 0.$$

2. A POSTERIORI ESTIMATORS WITH ERROR DOMINATED OSCILLATION

In order to gain some insight into our new approach we start with a formal splitting of the residual

$$\text{Res}(U) = f + \Delta U = \mathcal{P}_{\mathcal{M}} f + \Delta U + f - \mathcal{P}_{\mathcal{M}} f.$$

into an approximate *oscillation free residual* and *data oscillation*. From the first relation in (2) and a triangle inequality, we have reliability

$$\|u - U\|_{H_0^1(\Omega)} \lesssim \mathcal{E}(U, f, \mathcal{M}) + \text{osc}(f, \mathcal{M})$$

of the estimator $\mathcal{E}(U, f, \mathcal{M})^2 := \sum_{z \in \mathcal{V}} \|\mathcal{P}_{\mathcal{M}}f + \Delta U\|_{H^{-1}(\omega_z)}^2$ up to oscillation $\text{osc}(f, \mathcal{M})^2 := \sum_{z \in \mathcal{V}} \|f - \mathcal{P}_{\mathcal{M}}f\|_{H^{-1}(\omega_z)}^2$. We suppose that $\mathcal{P}_{\mathcal{M}} : H^{-1}(\Omega) \rightarrow H^{-1}(\Omega)$ is linear and make the following demands:

- **Error dominated oscillation:** For all $V \in \mathbb{V}(\mathcal{M})$ we have

$$(3) \quad \|f - \mathcal{P}_{\mathcal{M}}f\|_{H^{-1}(\omega_z)} \lesssim \|u - V\|_{H_0^1(\omega_z)}.$$

We first note that an error dominated oscillation implies local efficiency

$$\begin{aligned} \|\mathcal{P}_{\mathcal{M}}f + \Delta V\|_{H^{-1}(\omega_z)} &\leq \|f + \Delta V\|_{H^{-1}(\omega_z)} + \|f - \mathcal{P}_{\mathcal{M}}f\|_{H^{-1}(\omega_z)} \\ &\lesssim \|u - V\|_{H_0^1(\omega_z)}. \end{aligned}$$

If we choose $V \equiv 0$ in (3) then we have from the local efficiency that

$$(4) \quad \|\mathcal{P}_{\mathcal{M}}f\|_{H^{-1}(\omega_z)} \lesssim \|u\|_{H_0^1(\omega_z)} = \|f\|_{H^{-1}(\omega_z)},$$

i.e. $\mathcal{P}_{\mathcal{M}}$ is locally stable. Moreover, for $f = -\Delta V$, $V \in \mathbb{V}(\mathcal{M})$, we have $u = V$ and thus

$$(5) \quad \|f - \mathcal{P}_{\mathcal{M}}f\|_{H^{-1}(\omega_z)} \lesssim 0 \quad \Rightarrow \quad \Delta V = \mathcal{P}_{\mathcal{M}}\Delta V,$$

i.e. $\mathcal{P}_{\mathcal{M}}$ is locally invariant. Stability and invariance are in fact equivalent to the error domination (3), as can be seen from

$$\begin{aligned} \|f - \mathcal{P}_{\mathcal{M}}f\|_{H^{-1}(\omega_z)} &\leq \|f + \Delta V\|_{H^{-1}(\omega_z)} + \|\mathcal{P}_{\mathcal{M}}(\Delta V + f)\|_{H^{-1}(\omega_z)} \\ &\lesssim \|f + \Delta V\|_{H^{-1}(\omega_z)} \lesssim \|u - V\|_{H_0^1(\omega_z)}. \end{aligned}$$

- **Computability:** We need to have that $\mathcal{P}_{\mathcal{M}}f$ is computable and discrete, i.e. $\mathcal{E}(U, f, \mathcal{M})$ can be estimated from below and above in a computable manner. We say that $\mathcal{P}_{\mathcal{M}}f$ is computable if it can be determined from the information available in the linear systems for finite element approximations. To be more precise, for Φ denoting the span of all finite products of nodal basis functions, we assume that the evaluations

$$\langle f, \phi \rangle, \quad \phi \in \Phi, \quad \text{are known exactly.}$$

In order to have that the oscillation is potentially of higher order, we additionally demand that $\mathcal{P}_{\mathcal{M}}$ is invariant on piecewise constant functions; compare with (1).

Because of shortage of space, we cannot present our new approach satisfying all above demands here in detail. In a nutshell, its construction is based on the representation

$$\langle \mathcal{P}_{\mathcal{M}}f, v \rangle = \sum_{K \in \mathcal{M}} \int_K f_K v + \sum_{F \in \mathcal{F}} \int_F f_F v,$$

where \mathcal{F} is the set of all $d-1$ dimensional interelement faces of \mathcal{M} . The coefficients $f_K, f_F \in \mathbb{R}, K \in \mathcal{M}, F \in \mathcal{F}$ are determined by testing f with suitable locally supported element respective face bubble functions from Φ . Concluding, we have

$$\sum_{z \in \mathcal{V}} \|\mathcal{P}_{\mathcal{M}}f + \Delta U\|_{H^{-1}(\omega_z)}^2 + \|f - \mathcal{P}_{\mathcal{M}}f\|_{H^{-1}(\omega_z)}^2 \approx \|u - U\|_{H_0^1(\Omega)}^2.$$

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 H^{-1} -approximation with piecewise polynomials

FRANCESCA TANTARDINI

(joint work with Andreas Veerer, Rüdiger Verfürth)

We consider approximation in the H^{-1} -norm with continuous and discontinuous piecewise polynomials over a conforming triangulation of the domain $\Omega \subset \mathbb{R}^d$.

On the one hand, we aim at error estimates in terms of the local mesh-size and with minimal regularity assumptions, that can be used, for example, in the error estimation in the context of parabolic problems, where the error for the time derivative is often measured in a negative norm. On the other hand, we would like to prepare the basis for the application of the adaptive tree approximation algorithm of Binev and DeVore [2], which provides near-best approximations in the H^{-1} -norm.

To this end, we follow the ideas of [5], where it was proved that the global best error in the H^1 -seminorm is equivalent to the ℓ^2 -sum of local best errors on elements, when approximating with functions from a space S consisting of continuous piecewise polynomials:

$$(1) \quad \inf_{v \in S} \|\nabla(f - v)\|^2 \approx \sum_{K \in \mathcal{T}} \inf_{v_K \in S|_K} \|\nabla(f - v_K)\|_K^2.$$

This provides a better understanding of the approximation properties of the discrete space, allowing in particular to derive error estimates of optimal order in terms of piecewise regularity and to derive suitable indicators for the tree approximation algorithm.

A simple example shows that (1) cannot hold if the H^1 -seminorm is replaced by the H^{-1} -norm. In fact, consider the functional $\delta_F \in H^{-1}(\Omega)$ that takes the average of every test function $\varphi \in H_0^1(\Omega)$ over a face F of the triangulation, i.e. $\langle \delta_F, \varphi \rangle = \int_F \varphi$. Every local best error on the right-hand side vanishes, but the global best error does not. This holds even if we approximate with discontinuous piecewise polynomials. In fact, although the discrete space decouples, the global nature of the norm couples the approximations. There is indeed no set-additivity in the background of the H^{-1} -norm, and the norm on the union of two sets is in general not bounded by the norms on each set separately. Another counterexample shows that it is not possible to localize the best error in the H^{-1} -norm either on pairs of adjacent elements; one therefore has to consider bigger subdomains.

In the context of a posteriori error estimation, it has been proven that the H^{-1} -norm of the residual is equivalent to the ℓ^2 -sum of the H^{-1} -norms on finite element stars, i.e. the set of elements that share a vertex. Key ingredients are the fact that the basis functions of the conforming finite element space of lowest order form a partition of unity and have support on the stars around the vertices, and the orthogonality of the residual with respect to these functions.

In a similar fashion we exploit the same partition of unity to show that the interpolation error with respect to a suitable interpolation operator is bounded by the ℓ^2 -sum of the local H^{-1} -norms on stars around the vertices \mathcal{V} of the triangulation

$$(2) \quad \|f - \Pi_{\text{loc}} f\|_{-1}^2 \leq C \sum_{z \in \mathcal{V}} \|f\|_{-1; \omega_z}^2.$$

The constant $C > 0$ depends only on the dimension d and on the shape-parameter of the mesh. The localization operator may map onto various spaces, e.g., onto piecewise affine, globally continuous functions or onto piecewise constant functions. The adjoint operator maps however always onto piecewise affine and globally continuous functions, is locally invariant onto constants and allows for local Poincaré inequalities, property that leads to (2).

We apply this result to $f - \Pi f$, where Π is an invariant and locally stable interpolation operator, whose local features permit to bound the interpolation error on a star by means of the best errors on the stars in the neighborhood. We therefore prove that the best error can be localized to the stars around the vertices:

$$(3) \quad \inf_{v \in S} \|f - v\|_{-1}^2 \approx \sum_{z \in \mathcal{V}} \inf_{v_z \in S|_{\omega_z}} \|f - v_z\|_{-1; \omega_z}^2.$$

Here S may be the space of continuous or discontinuous piecewise polynomials of arbitrary order. Moreover, we can prove the same result also for the space of functionals in $H^{-1}(\Omega) \setminus L^2(\Omega)$ that average over the faces of the triangulation.

As an application, we derive a priori error estimates of optimal order in terms of the local mesh-size and local regularity. The additional regularity is measured with a scale of Hilbert spaces: Integer regularity is measured in the standard Sobolev spaces $H^r(\omega_z)$, while fractional regularity is measured with a suitably weighted interpolation norm, see [3]. In this way the result is robust with respect to the parameter that measures the intermediate regularity between two integer orders.

The localization result in the form (3) is not yet useful for deriving local indicators for the tree approximation algorithm. In fact, for every element K , the indicator related to K has to depend only on K , and not on the neighboring elements. A combination of the local best errors on the stars around the vertices of K does not satisfy this property. Therefore, we need a modification of (3), involving e.g. minimal stars in the spirit of minimal pairs or minimal rings as in [1, 4].

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Adventures in Adaptivity

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(joint work with Randolph E. Bank)

1. INTRODUCTION

Let $H(\Omega)$ denote a Sobolev space of interest, equipped with norm $\|\cdot\|_\Omega$, and let $\mathcal{S}_h \subset H$ denote a finite element space, associated with a tessellation \mathcal{T}_h of Ω . In [3], it was shown that under weak assumptions

$$(1) \quad \|u - \mathcal{I}u\|_\Omega \leq C\|u - v\|_\Omega$$

$$(2) \quad \|u - \mathcal{I}u\|_t \leq C\|u - v\|_t$$

for all $v \in \mathcal{S}_h$. Here $u \in H$, $\mathcal{I}u \in \mathcal{S}_h$ is the usual interpolant of u , $t \in \mathcal{T}_h$, and $\|\cdot\|_t$ is the norm restricted to element t . In finite element analysis, interpolation error $u - \mathcal{I}u$ is often used as an upper bound for the error in various finite element approximations, here denoted $u_h \in \mathcal{S}_h$. Estimates (1)-(2) provide lower bounds for the error for *any* finite element approximation. Thus these bounds can be combined with the usual a priori estimates for u_h to see that

$$(3) \quad C_1\|u - \mathcal{I}u\|_\Omega \leq \|u - u_h\|_\Omega \leq C_2\|u - \mathcal{I}u\|_\Omega$$

$$(4) \quad C_3\|u - \mathcal{I}u\|_t \leq \|u - u_h\|_t$$

In this work, we explore the practical implications of (3)-(4) in the context of adaptive finite element methods, and in particular h -adaptive and hp -adaptive feedback loops.

Inequalities (3)-(4) show that interpolation error is both efficient and reliable [4, 5] for controlling an adaptive feedback loop of the type commonly employed in adaptive finite element calculations for solving partial differential equations. While interpolation error cannot in general be used for an a posteriori error estimate, in this work we create an environment based on interpolation error that allows us to study and evaluate various adaptive approaches independently of the PDE. Aspects such as approximate solution of linear and nonlinear systems, unknown exact solutions, and the a posteriori error estimation procedure make it difficult to focus exclusively on the adaptive procedure itself. Using interpolation error, we construct idealized “reference” adaptive procedures. We then employ these reference procedures to compare and evaluate various approaches. Indeed, during the course of our investigations, we analyzed and improved the adaptive approach used in the PLTMG software package [1]. The version described in this summary

work is not the procedure in the currently available version of PLTMG (although it is quite similar), but it or its descendant will appear in future versions of the package.

We are also able to study the effectiveness of certain a posteriori error estimates within this environment. In particular, we compare the behavior of some fixed adaptive algorithm using interpolation error for the local error indicators with the same adaptive algorithm using some computable a posteriori error estimate for the the local error indicators. In this case, the observed differences can be attributed to the a posteriori error estimate.

While we think the results for various adaptive approaches are by themselves quite interesting, and reveal the advantages and disadvantages of the given approaches, we also believe that our general methodology for evaluating the different approaches is an equally important contribution.

2. METHODOLOGY

We ran experiments on three different problems, chosen to exhibit typical challenges encountered by adaptive methods. In these experiments we enriched the finite element subspace using several h and hp adaptive strategies. The local error indicators used in these adaptive methods were either the interpolation error for the exact solution or error indicators generated by recovering derivatives using the interpolant as a proxy for the finite element solution. The recovery procedure is described in detail in [2]. In all experiments we started from an initial mesh of eight elements and refined the mesh to one containing approximately 250,000 degrees of freedom.

Adaptive refinement is implemented by an iterative process with a three step feedback inner loop

$$(5) \quad \text{solve} \rightarrow \text{estimate} \rightarrow \text{refine}$$

In our methodology, the “solve” steps are skipped and we use the interpolant in place of the finite element solution. For each experiment we provide many data items. After each iteration, we compute the error

$$\text{error} = \frac{\|\nabla(u - \mathcal{I}_p u)\|_\Omega}{\|\nabla u\|_\Omega}$$

and we approximate the cumulative computational effort with

$$\text{effort}_{1.5} = \sum_{k=1}^L N_k^{1.5}$$

where L is the number of iterations completed and N_k is the number of degrees of freedom at step k . We also provide the order of convergence for each experiment.

3. CONCLUSION

Our general methodology proves effective in evaluating adaptive strategies and a posteriori error estimators. The various data items provide insights that help

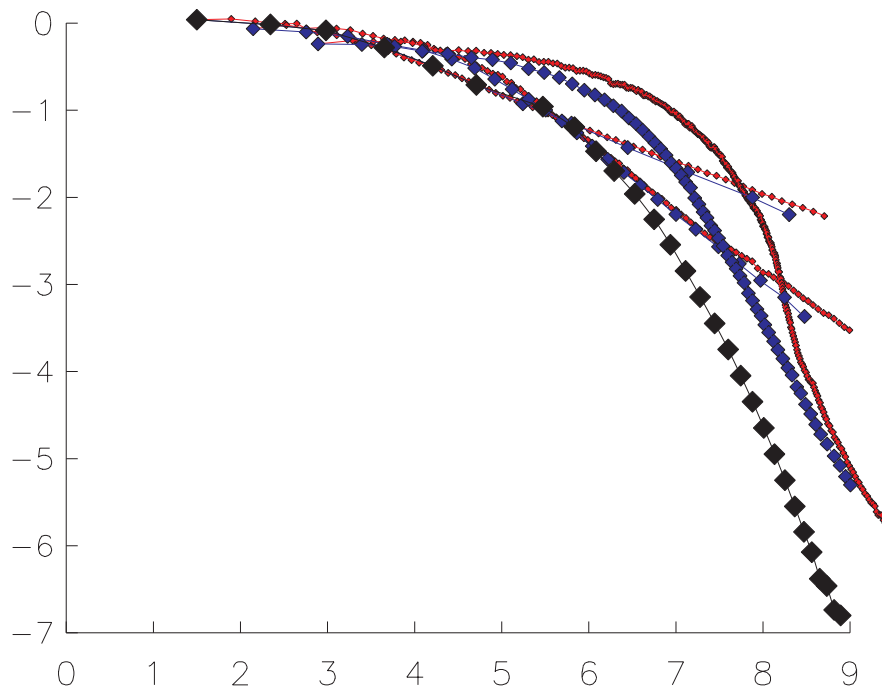


FIGURE 1. Log effort versus log error. PLTMG hp method (large squares), PLTMG h method for $p = 1, 2, 4$ (medium squares), Common marking method $\theta = .5$ for $p = 1, 2, 4$ (small squares).

improve refinement strategies and error estimators. Our effort indicator allows us to compare the efficiency of different adaptive strategies. From the plots of $\log_{10}(\text{effort}_{1.5})$ versus $\log_{10}(\text{error})$, we observe three interesting conclusions. First, on all three problems, the PLTMG refinement scheme is more efficient than the common marking scheme. This is most likely because PLTMG allows a single element to be refined multiple times during one adaptive inner loop. Second, hp -refinement is more efficient than h -refinement for all problems. Third, when using hp -refinement, the test to decide whether to refine in h or p is very important for the overall efficiency.

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A posteriori estimates for the Laplace-Beltrami operator on C^2 surfaces

ALAN DEMLOW

(joint work with Andrea Bonito)

In this talk we discuss construction of practical and computationally efficient algorithms for solving the Laplace-Beltrami problem on a C^2 surface γ . Such a surface may be represented as the level set of a distance function which gives rise to a closest-point projection onto γ . Well-known a priori error estimate indicate that when a finite element method of polynomial degree r is defined on a approximation to γ of polynomial degree k , the resulting energy error is of order $h^r + h^{k+1}$. The former $O(h^k)$ error term is a standard Galerkin error. The latter $O(h^{k+1})$ term arises from the consistency error due to the surface approximation and is often called a geometric error. It is in effect superconvergent by one order due to special orthogonality properties of the closest point projection. A posteriori error estimates for this setting were given in [2]. These similarly measure the Galerkin error using residual a posteriori error estimators and the geometric consistency error using computable information. A major drawback of the geometric consistency a posteriori error estimators in this approach is that they require computation of the closest point projection and corresponding information, which is often not conveniently available in practice.

A more recent approach to a posteriori error estimation for the Laplace-Beltrami problem was given in [1]. This approach allows for more general parametric surface representations as well as $C^{1,\alpha}$ surfaces. Both of these generalizations are desirable in practical situations. However, the geometric error estimators used in this approach are only of order h^k and thus do not take advantage of the superconvergence properties of the closest point projection when γ is C^2 .

In our work we construct new geometric a posteriori error estimators for C^2 surfaces which allow for reasonably generic parametric surface representations while taking advantage of the closest point projection in order to preserve the $O(h^{k+1})$ order of the geometric error. Computational examples demonstrate that they sometimes yield large efficiency gains compared with the approach of [1] when implemented in AFEM, and that less surface regularity is required to achieve optimal convergence rates so long as γ is at least C^2 .

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**A new trace inequality and its applications in robust error estimates
for discontinuous finite element approximations**

SHUN ZHANG

(joint work with Zhiqiang Cai, Cuiyu He, Purdue University)

In this talk, we present robust a priori and a posteriori error estimates of various discontinuous finite element approximations to the interface problem:

$$(1) \quad -\nabla \cdot (\alpha(x)\nabla u) = f \quad \text{in } \Omega, \quad u = 0 \quad \text{on } \partial\Omega.$$

Here, $f \in L^2(\Omega)$ is a given function; and the diffusion coefficient $\alpha(x) > 0$ is piecewise constant with possible large jumps across subdomain boundaries (interfaces). It is well-known that the solution of problem (1) is only in $H^{1+s}(\Omega)$ with possible very small $s > 0$.

For the conforming finite element approximation to problem (1), it is proved (see, e.g., [2]) that the a priori error estimate in the energy norm is robust with respect to the diffusion coefficient, i.e., the constant in the error bound is independent of the jump of the diffusion coefficient. Moreover, under an assumption on the distribution of the diffusion coefficient, i.e., the so-called Quasi-Monotonicity Assumption (QMA), it is shown (see, e.g., [2, 6]) that the residual a posteriori error estimate is robust as well. However, the QMA is restrictive, and numerical results by many researchers suggest that it is not needed.

For the Crouzeix-Raviart (CR) nonconforming and the discontinuous Galerkin finite element approximations to problem (1) in both two and three dimensions, we are able to show in [4] that both the a priori and the residual a posteriori error estimates are robust with respect to the diffusion coefficient and that the a priori estimates are also optimal with respect to local regularity of the solution. Moreover, these estimates are obtained without the QMA. The robust and local optimal a priori estimates are established through proving a robust Céa's Lemma type of results for the CR nonconforming and the discontinuous elements. The robust reliability bound of the residual a posteriori error estimator without the QMA is obtained through a new and direct analysis developed in [3]. Unlike the standard approach, our analysis does not require the Helmholtz decomposition. Additional and critical tool needed for the above mentioned results is our recently proved trace inequality stated below.

Let \mathcal{T} be a regular triangulation of the domain Ω , K be an element in \mathcal{T} , F be a face of the element K , and $s > 0$ be a fixed real number. Assume that v is a given function in $H^{1+s}(K)$ and that Δv is in $L^2(K)$, where Δ is the Laplace operator. Then there exists a small $0 < \delta < \min\{s, 1/2\}$, depending on v , and a positive constant C independent of δ such that the following trace inequality:

$$\|\nabla v \cdot \mathbf{n}\|_{\delta-1/2, F} \leq C (\|\nabla v\|_{0, K} + h_K \|\Delta v\|_{0, K})$$

holds. This inequality improves the following inequality derived in [1, 5].

$$\|\nabla v \cdot \mathbf{n}\|_{\delta-1/2, F} \leq C (\|\nabla v\|_{\delta, K} + h_K^{1-\delta} \|\Delta v\|_{0, K}).$$

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Two-sided bounds on eigenvalues of elliptic operators

TOMÁŠ VEJCHODSKÝ

The standard conforming approximations of Galerkin type provide natural upper bounds on eigenvalues of symmetric elliptic operators. In this talk we address the problem of computing the corresponding lower bounds. This problem has been studied for many decades, see for example [11, 12, 13, 18, 20]. Recent successful approaches to compute guaranteed lower bounds include methods based on both nonconforming [5, 6, 8, 9, 10] and conforming [2, 14, 17] finite elements.

Several classical approaches, see for example a review in [16], provide lower bounds on eigenvalues for an abstract operator A defined on a Hilbert space H . Straightforward practical implementation of these methods requires to evaluate Au for some $u \in H$. If A is a second-order elliptic partial differential operator defined on a domain Ω then Au corresponds to its evaluation in the strong (pointwise) sense and, hence, it requires the corresponding Sobolev regularity $u \in H^2(\Omega)$. This regularity is, however, higher than the natural $H^1(\Omega)$ regularity of the weak solution and the standard finite element trial functions.

In this contribution, we consider the classical Weinstein’s [20] and Kato’s [11] bounds and show how to modify them to obtain the lower bounds on eigenvalues for the natural $H^1(\Omega)$ regularity of trial functions.

The presented method can be applied to eigenvalue problems for general symmetric elliptic second-order partial differential operators. However, for the simplicity of presentation, we consider here only the Laplace eigenvalue problem

$$-\Delta u_i = \lambda_i u_i \quad \text{in } \Omega, \quad u_i = 0 \quad \text{on } \partial\Omega,$$

where the domain $\Omega \subset \mathbb{R}^2$ is assumed to be Lipschitz. Introducing the space $V = H_0^1(\Omega)$, the weak formulation reads: find $u_i \in V \setminus \{0\}$ and $\lambda_i \in \mathbb{R}$ such that

$$(1) \quad a(u_i, v) = \lambda_i b(u_i, v) \quad \forall v \in V,$$

where $a(u, v) = (\nabla u, \nabla v)$, $b(u, v) = (u, v)$ and (\cdot, \cdot) denotes the $L^2(\Omega)$ inner product. It is well known that there exist a countable sequence of eigenvalues

$0 < \lambda_1 \leq \lambda_2 \leq \dots$ and the corresponding eigenfunctions can be normalized such that $b(u_i, u_j) = \delta_{ij}$.

The generalization of the classical Weinstein's bound to the weak setting is formulated as follows.

Theorem 4. *Let $u_* \in V \setminus \{0\}$ and $\lambda_* \in \mathbb{R}$ be arbitrary and let the closeness condition*

$$(2) \quad \sqrt{\lambda_{n-1}\lambda_n} \leq \lambda_* \leq \sqrt{\lambda_n\lambda_{n+1}}$$

hold. Let $w \in V$ be given by

$$(3) \quad a(w, v) = a(u_*, v) - \lambda_* b(u_*, v) \quad \forall v \in V.$$

and let there exist $\eta > 0$ such that $\|w\|_a \leq \eta$. Then

$$(4) \quad \ell_n \leq \lambda_n, \quad \text{where} \quad \ell_n = \frac{1}{4\|u_*\|_b^2} \left(-\eta + \sqrt{\eta^2 + 4\lambda_*\|u_*\|_b^2} \right)^2.$$

Lower bound (4) is quite robust and general, but its speed of convergence is linear in terms of η , which is suboptimal. However, using a more involved technique, we can generalize the classical Kato's bound to the weak setting and obtain a quadratically convergent lower bound.

Theorem 5. *Let $u_* \in V \setminus \{0\}$ be arbitrary and let $\lambda_* = \|u_*\|_a^2 / \|u_*\|_b^2$. Let there be $\nu > 0$ such that*

$$(5) \quad \lambda_{n-1} < \lambda_* < \nu \leq \lambda_{n+1}$$

for a fixed index n . If w is given by (3) and $\|w\|_a \leq \eta$ then

$$(6) \quad L_n \leq \lambda_n, \quad \text{where} \quad L_n = \lambda_* \left(1 + \frac{\nu}{\lambda_*(\nu - \lambda_*)} \frac{\eta^2}{\|u_*\|_b^2} \right)^{-1}.$$

Practically, we solve the eigenvalue problem (1) numerically using the standard conforming finite element method. We introduce the standard finite element triangulation \mathcal{T}_h of Ω , the space $V_h = \{v_h \in V : V_h|_K \in P_1(K) \ \forall K \in \mathcal{T}_h\}$, and look for $\lambda_{h,i} > 0$ and $u_{h,i} \in V_h \setminus \{0\}$ such that

$$a(u_{h,i}, v_h) = \lambda_{h,i} b(u_{h,i}, v_h) \quad \forall v_h \in V_h.$$

It is well known that $\lambda_{h,i}$ provide upper bounds on λ_i . To evaluate lower bounds (4) and (6), we need to find a tight bound η on the energy norm $\|w\|_a$. This we do by using the complementarity (or two-energy) principle, see e.g. [3].

Theorem 6. *If $\mathbf{q} \in \mathbf{H}(\text{div}, \Omega)$ satisfies $-\text{div } \mathbf{q} = \lambda_* u_*$ and if $\eta = \|\nabla u_* - \mathbf{q}\|$ then $\|w\|_a \leq \eta$.*

The flux reconstruction \mathbf{q} can be in practice constructed in various ways, see e.g. [1, 7, 19]. We employ the local and efficient approach introduced in [4].

The presented lower bounds on eigenvalues are suitable for a wide class of symmetric elliptic eigenvalue problems with mixed Dirichlet, Neumann, and Robin boundary conditions. They utilize the standard conforming finite element technology and the computed error estimator η can be straightforwardly used in adaptive

algorithms for both local mesh refinement and reliable stopping criterion. Both (4) and (6) are given by simple formulas. We proposed to compute both of them and use the more accurate one. The bound (6) is quadratically convergent and provides more accurate values on fine meshes, but numerical experiments confirm that the linearly convergent bound (4) is often more accurate on rougher meshes.

The bound (6) requires the quantity ν satisfying (5). This condition however cannot be verified unless a lower bound on λ_{n+1} is known. In [15] a homotopy method to compute a (rough) lower bound on λ_{n+1} is proposed. However, if the lower bound (6) is not required to be guaranteed (in the mathematical sense) then it is natural to set $\nu = \ell_{n+1}$ computed by (4). Numerical experiments indicate that as soon as $\lambda_{h,n} < \ell_{n+1} \leq \lambda_{h,n+1} < \ell_{n+2}$ and $\lambda_{h,n+1} \leq \sqrt{\ell_{n+1}\ell_{n+2}}$ then we can have a high confidence that hypotheses of Theorem 4 are satisfied and $\ell_{n+1} \leq \lambda_{n+1}$. Consequently, we can be confident about condition (5) for $\lambda_* = \lambda_{h,n}$ and $\nu = \ell_{n+1}$ and, hence, about the bound (6).

Practically, the performance of the bound (6) is limited by the spectral gap $\lambda_{n+1} - \lambda_n$ due to the factor $\nu - \lambda_*$. To solve this issue, we will concentrate on the case of tightly clustered and multiple eigenvalues in our future work.

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Auxiliary subspace techniques as a general-purpose approach for a posteriori error estimation

JEFFREY S. OVALL

(joint work with Harri Hakula, Michael Nielan)

The auxiliary subspace approach for estimating finite element discretization error is based on the solution of a global residual equation in a properly-chosen auxiliary space of functions, involving the same bilinear form used for computing the finite element approximation. The original variational problem, the finite element approximation problem, and error approximation problem have the general forms:

- Find $u \in \mathcal{H}$ such that $B(u, v) = F(v)$ for all $v \in \mathcal{H}$,
- Find $\hat{u} \in V$ such that $B(\hat{u}, v) = F(v)$ for all $v \in V$,
- Find $\varepsilon \in W$ such that $B(\varepsilon, v) = \underbrace{F(v) - B(\hat{u}, v)}_{B(u-\hat{u}, v)}$ for all $v \in W$,

where the bilinear form B and the linear functional F are derived from some second-order linear elliptic boundary value problem on a bounded domain $\Omega \subset \mathbb{R}^d$, and \mathcal{H} is some appropriate closed subspace of $H^1(\Omega)$. The spaces V and W are finite dimensional subspaces of \mathcal{H} , with V being a standard finite element approximation space—say continuous piecewise-polynomial functions on a conforming partition of Ω into simplicial and/or tensorial cells—and $V \cap W = \{0\}$. If B happens to be an inner-product, then ε is clearly the corresponding orthogonal projection of the error $u - \hat{u}$ onto the space W . If B is merely coercive, it is trivial to see that $\|\varepsilon\|_{\mathcal{H}}$ provides, up to a constant, a lower bound on $\|u - \hat{u}\|_{\mathcal{H}}$.

In traditional hierarchical basis-type schemes (cf. [1]) and references therein), the space W is chosen so that $V \oplus W$ is a standard approximation space that is “richer” than V in terms of its ability to approximate the solution u . We take a different view of the role of W , namely that it should have degrees of freedom that allow it to adequately “capture” the two key components of the approximation error,

- The volumetric residuals R_T that express how the finite element function \hat{u} fails to satisfy the strong form of the PDE on the cell T ,
- The face residuals r_F that express how the finite element function fails to have a continuous flux across interfaces F between cells, or how it fails to satisfy natural boundary conditions on boundary faces F .

For problems in 2D, the approach we advocate is typically the same as the traditional hierarchical basis approach, but the two approaches differ in three (or higher) dimensions. In brief, we propose that W should be spanned by “cell bubbles” and “face bubbles” that provide the new degrees of freedom we seek. Our analysis shows that $\|\varepsilon\|_{\mathcal{H}}$ provides an upper-bound on $\|u - \hat{u}\|_{\mathcal{H}}$, up to a constant and a residual oscillation term that is designed to be of higher order, and is thus typically ignored in practical computations, but is nonetheless explicitly computable, and so can be incorporated if desired. We also argue that the matrix for computing ε is much better behaved than its counterpart for computing \hat{u} , with a diagonal rescaling of the former being all that is necessary to resolve the system using a fixed small number of iterations of a simple scheme like conjugate gradients or GMRES.

Extensive experiments on a wide range of problems, including those having discontinuous and high-contrast diffusion coefficients, and those for which convection is dominant, demonstrate the robustness of h , p and hp -versions of the method, both as a driver of automatic refinement, and as an estimate of the actual error. In all of these experiments, the ratio of error and error estimates remained stable regardless of which version of refinement was used, and the error estimate was nearly always within a factor of two of the actual error, indicating robustness for many realistic problems. Some theoretical issues that remain open at this stage are:

- The analysis for the upper bound on the error allows that the constant appearing in this bound could depend on the degree of polynomials used in the discretization. Experiments indicate that this is probably not the case.
- The constants that establish the equivalence of error and error estimate (in an appropriate energy norm) could potentially depend on the contrast between the diffusion and convection coefficients for convection-dominated problems. The performance of the estimator in the moderate convection dominance, where it is not necessary to resort to alternate discretization schemes, is much better than can be explained by the current analysis.
- Even for basic problems like the Poisson problem in 2D, there is no proof that typical refinement schemes will lead to convergent adaptive algorithms when this class of estimator is used to mark cells for refinement. The empirical evidence strongly suggests that this approach will perform at least as well those for which proofs have been given.

The theoretical results, and experiments using h -refinement with polynomials of degree ≥ 1 , p -refinement and hp -refinement are taken from [2]. The lowest-order experiments in 3D are taken from [3]. The experiments demonstrating asymptotic

exactness in the lowest order case, as well as effectivities in other norms, have not appeared in the presented form in any publication; theoretical justification of these results can be found in [5, 4].

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An adaptive FEM for linear elliptic equations in nondivergence form with Cordes coefficients

DIETMAR GALLISTL

Let $\Omega \subseteq \mathbb{R}^d$ be an open, bounded, convex polytope for $d \in \{2, 3\}$. The numerical approximation of strong solutions $u \in H_0^1(\Omega) \cap H^2(\Omega)$ to the second-order elliptic partial differential equation

$$\sum_{j,k=1}^d A_{jk} \partial_{jk}^2 u = f \quad \text{in } \Omega \quad u = 0 \quad \text{on } \partial\Omega$$

(where $f \in L^2(\Omega)$ is a given square-integrable function) with conventional schemes suffers from the difficulty that the problem is not posed in divergence form. In the case that the coefficient $A \in L^\infty(\Omega; \mathbb{R}^{d \times d})$ satisfies the Cordes condition, unique existence of strong solutions was established in [3]. This contribution, which is based on the work [2], discusses an equivalent reformulation of the PDE as a variational fourth-order problem, namely

$$\operatorname{div} \operatorname{div} \left(\sum_{j,k=1}^d A_{jk} \partial_{jk}^2 u A \right) = \operatorname{div} \operatorname{div} (f A) \quad \text{in } H^{-2}(\Omega)$$

subject to the boundary conditions

$$u = 0 \quad \text{and} \quad \left(\sum_{j,k=1}^d A_{jk} \partial_{jk}^2 u A \right)_{nn} = 0 \quad \text{on } \partial\Omega$$

(n denoting the outer unit normal). This problem resembles the model of the simply supported Kirchhoff-Love plate from linear elasticity theory, and known standard finite element techniques for variational problems in subspaces of H^2 can be utilized for its numerical approximation. Alternatively, mixed finite element methods [1] can be employed. Besides immediate quasi-optimal a priori error

bounds, the variational setting allows for a posteriori error control with explicit constants and adaptive mesh-refinement. The convergence of an adaptive algorithm can be proved and empirical observations in numerical experiments suggest that its convergence rate may be of optimal order.

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Regularized adaptive finite element methods for nonmonotone quasilinear PDE

SARA POLLOCK

The numerical approximation of quasilinear partial differential equations of the form $-\operatorname{div}(\kappa(u)\nabla u) = f$, in domain Ω , can pose unique challenges not encountered in the analogous linear or semilinear diffusion problems, or even in quasilinear problems of monotone type. In particular, thin internal layers and steep gradients in the *a priori* unknown diffusion coefficient $\kappa(u)$, may need to be uncovered as the solution process progresses. Starting the simulation on a coarse mesh, nonuniform recovery of this coefficient can cause the divergence; or, the failure of convergence to physical solutions, of standard sequences of linearized problems used to approximate the solution of a suitably posed discrete nonlinear problem.

In this talk we first discuss applications of the stationary diffusion problem, and motivate its efficient and accurate solution. We then discuss the current state of the theory; namely, local well posedness and approximation properties of the adaptive finite element solution, as in [1, 2], assuming a fine-enough initial mesh condition and a close enough initial guess to start the iterative process on each mesh partition. We then discuss how these assumptions make the solution process computationally infeasible, even for simple model problems.

An auto-adaptive regularization technique is then introduced, combining the techniques of Tikhonov regularization and pseudo-time stepping, as described by the author in [3]; a generalized Newmark time-integration strategy, as discussed in [4]; and an inexact regularization technique, as in [5].

Finally, we discuss some particular assignments of regularization parameters based on computable quantities at each iteration of the method. An adaptive algorithm is introduced to assign updates to regularization parameters and define criteria for inexact solves, while adaptively refining the mesh. The ideas are illustrated with numerical examples of a model problem.

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An optimal AFEM for higher-order problems

MIRA SCHEDENSACK

This talk considers new mixed finite element methods (FEMs) for problems of the form: Seek $u \in H_0^m(\Omega)$ with

$$(-1)^m \Delta^m u = f$$

for arbitrary $m = 1, 2, 3, \dots$. The mixed FEMs are based on a new mixed formulation, which decomposes a function $\varphi \in H(\operatorname{div}, \Omega)$ with $(-1)^m \operatorname{div}^m \varphi = f$ in the m th derivative $D^m u$ of the solution u and a symmetric part of a Curl of a tensor-valued H^1 function. The new mixed FEMs approximate directly the m th derivative $\sigma = D^m u$ of the solution u and therefore allow for lowest-order approximations, i.e., piecewise constants for the approximation of $D^m u$ and piecewise affine functions for the approximation of the Lagrange multiplier.

The discrete problem seeks $(\sigma_h, \alpha_h) \in P_k(\mathcal{T}; \mathbb{S}(m)) \times Y(\mathcal{T})$ with

$$\begin{aligned} (\sigma_h, \tau_h)_{L^2(\Omega)} + (\tau_h, \operatorname{sym} \operatorname{Curl} \alpha_h)_{L^2(\Omega)} &= (\varphi, \tau_h)_{L^2(\Omega)} && \text{for all } \tau_h \in P_k(\mathcal{T}; \mathbb{S}(m)) \\ (\sigma_h, \operatorname{sym} \operatorname{Curl} \beta_h)_{L^2(\Omega)} &= 0 && \text{for all } \beta_h \in Y(\mathcal{T}), \end{aligned}$$

where $P_k(\mathcal{T}; \mathbb{S}(m))$ denotes the space of piecewise polynomials of degree $\leq k$ with values in the symmetric tensors and $Y(\mathcal{T}) \subseteq P_{k+1}(\mathcal{T}; \mathbb{S}(m-1)) \cap H^1(\Omega; \mathbb{S}(m-1))$ consists of piecewise polynomials of degree $\leq k+1$ which are globally continuous and satisfy some constraints to ensure uniqueness of the solution.

For $m = 2$ and $k = 0$, a discrete Helmholtz decomposition of [1] proves that the space of *discrete gradients* defined by

$$(1) \quad W(\mathcal{T}) := \{ \tau_h \in P_k(\mathcal{T}; \mathbb{S}(m)) \mid \forall \beta_h \in Y(\mathcal{T}) : (\tau_h, \operatorname{sym} \operatorname{Curl} \beta_h)_{L^2(\Omega)} = 0 \}$$

equals the space of non-conforming Hessians of Morley finite element functions [3].

Let $\Pi_{P_k(\mathcal{T};\mathbb{S}(m))}$ denote the L^2 projection onto $P_k(\mathcal{T};\mathbb{S}(m))$ and $\mathcal{E}(T)$ denote the set of edges of a triangle $T \in \mathcal{T}$. The residual based error estimators

$$\begin{aligned}\lambda^2(T) &:= \|h_T \operatorname{curl}_{\text{NC}} \sigma_h\|_{L^2(T)}^2 + h_T \sum_{E \in \mathcal{E}(T)} \|[\sigma_h \cdot \tau_E]_E\|_{L^2(E)}^2, \\ \mu^2(T) &:= \|\operatorname{sym}(\varphi) - \Pi_{P_k(\mathcal{T};\mathbb{S}(m))} \operatorname{sym}(\varphi)\|_{L^2(T)}^2, \\ \eta^2 &:= \sum_{T \in \mathcal{T}} (\lambda^2(T) + \mu^2(T))\end{aligned}$$

are reliable and efficient in the sense that there exist constants C_{eff} and C_{rel} with

$$C_{\text{eff}}^{-2} \eta^2 \leq \|\sigma - \sigma_h\|_{L^2(\Omega)}^2 + \|\operatorname{sym} \operatorname{Curl}(\alpha - \alpha_h)\|_{L^2(\Omega)}^2 \leq C_{\text{rel}}^2 \eta^2.$$

An adaptive algorithm based on separate marking and driven by the error estimators λ and μ yields optimal convergence rates in the sense that the output of the adaptive algorithm $(\mathcal{T}_\ell, \sigma_\ell, \alpha_\ell)$ satisfies

$$\begin{aligned}(2) \quad & (\operatorname{card}(\mathcal{T}_\ell) - \operatorname{card}(\mathcal{T}_0))^s (\|\sigma - \sigma_\ell\|_{L^2(\Omega)} + \|\operatorname{sym} \operatorname{Curl}(\alpha - \alpha_\ell)\|_{L^2(\Omega)}) \\ & \leq C \sup_{N \in \mathbb{N}_0} N^s \inf_{\mathcal{T} \in \mathbb{T}(N)} (\|\sigma - \Pi_{P_k(\mathcal{T};\mathbb{S}(m))} \sigma\|_{L^2(\Omega)} \\ & \quad + \inf_{\beta_{\mathcal{T}} \in Y(\mathcal{T})} \|\operatorname{sym} \operatorname{Curl}(\alpha - \beta_{\mathcal{T}})\|_{L^2(\Omega)} + \|\varphi - \Pi_{P_k(\mathcal{T};\mathbb{S}(m))} \varphi\|_{L^2(\Omega)}).\end{aligned}$$

Here, $\mathbb{T}(N)$ denotes the set of all conforming triangulations with at most N additional elements that can be created from the initial triangulation by newest-vertex bisection. The proof employs the abstract framework of [2]. To this end, discrete reliability and quasi-orthogonality have to be proved. The main ingredient in these proofs is the following projection property: Given a refinement \mathcal{T}_\star of \mathcal{T} and a *discrete gradient* $\tau_\star \in W(\mathcal{T}_\star)$, where $W(\mathcal{T}_\star)$ is defined in (1), the L^2 projection onto $P_k(\mathcal{T};\mathbb{S}(m))$ is a *discrete gradient* on the coarse triangulation \mathcal{T} , i.e., $\Pi_{P_k(\mathcal{T};\mathbb{S}(m))} \tau_\star \in W(\mathcal{T})$. Therefore, the solution $\sigma_{\mathcal{T}_\star}$ on a fine triangulation \mathcal{T}_\star can be used as a test function on a coarser triangulation \mathcal{T} without getting an additional Lagrange multiplier, but only with a modified right-hand side, i.e.,

$$(\sigma_{\mathcal{T}}, \sigma_{\mathcal{T}_\star})_{L^2(\Omega)} = (\Pi_{P_k(\mathcal{T};\mathbb{S}(m))} \varphi, \sigma_{\mathcal{T}_\star})_{L^2(\Omega)}.$$

The complete proof of the optimal convergence rates in (2) can be found in [4].

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Some New Robust *A Posteriori* Error Estimators for Singularly Perturbed Problems

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(joint work with Shaohong Du)

This report includes three results.

1) A new robust residual type *a posteriori* error estimator is developed and analyzed for convection-diffusion equations. A novel dual norm is introduced, under which the error estimator is proved to be robust with respect to the singularly perturbed parameter ϵ . Both theoretical and numerical results showed that the estimator performs better than the existing ones in literature.

2) We develop robust recovery-based *a posteriori* error estimators for streamline up-wind/Petrov Galerkin (SUPG) method for singularly perturbed convection-diffusion-reaction equations in a weak norm presented in 1). The flux is recovered by either local averaging in conforming $H(\text{div})$ spaces or weighted global L^2 -projection onto conforming $H(\text{div})$ spaces. Moreover, based on the recovered $H(\text{div})$ flux, we introduce a recovery stabilization procedure, and develop completely robust *a posteriori* error estimators with respect to the singular perturbation parameter. Numerical experiments are reported to support our theoretical results and to show the efficiency of the proposed estimators.

3) We consider mixed finite element approximation of a singularly perturbed fourth-order elliptic problem with two different boundary conditions, and present a new measure of the error, whose components are balanced with respect to the singular perturbation parameter. Robust residual-based *a posteriori* estimators for the new measure are obtained. This is achieved via a novel analytical technique based on an approximation result. Numerical experiments support our theory.

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Adaptive aggregation on graphs

LUDMIL ZIKATANOV

(joint work with Wenfang Xu, Jinchao Xu)

INTRODUCTION

We generalize some of the functional (hyper-circle) a posteriori estimates from finite element settings to general graphs and Hilbert space settings. We provide several theoretical results in regard to the generalized a posteriori error estimators. We use these estimates to construct aggregation based coarse spaces and multilevel solvers for graph Laplacians. The estimator is used to assess the quality of an aggregation adaptively. Furthermore, a reshaping algorithm based on this estimator is tested on several numerical examples.

Given a combinatorial graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, let $V = \mathbb{R}^{|\mathcal{V}|}$ and $\mathbf{W} = \mathbb{R}^{|\mathcal{E}|}$ be the vertex and edge spaces of \mathcal{G} , respectively. We consider $A \in \mathbb{R}^{n \times n}$ defined via

$$(Au, v) = \sum_{(i,j) \in \mathcal{E}} -a_{ij}(u_i - u_j)(v_i - v_j), \quad \forall u, v \in V,$$

where the sum runs over all edges $e = (i, j) \in \mathcal{E}$. The resulting matrix is known as the weighted Graph Laplacian of \mathcal{G} . In this talk we are interested in good approximations of the above bilinear form on a smaller subspace.

Define $G: V \rightarrow \mathbf{W}$ and $D: \mathbf{W} \rightarrow \mathbf{W}$ as follows: for $v \in V$, $\boldsymbol{\tau} \in \mathbf{W}$ we set $(Gv)_e = v_{\text{head}} - v_{\text{tail}}$, $(D\boldsymbol{\tau})_e = a_e \boldsymbol{\tau}_e$, $a_e = -a_{ij}$. The graph Laplacian then is $(Au, v) = (DGv, Gv)$. If $D = I$ we have the so called standard graph Laplacian.

An aggregation of \mathcal{G} is a splitting of the vertices into clusters, each cluster called an aggregate. We denote an aggregate by \mathcal{A} , its set of vertices by $\mathcal{V}_{\mathcal{A}}$ and the set of interior edges by $\mathcal{E}_{\mathcal{A}}$. For any two aggregates \mathcal{A} and \mathcal{A}' , denote by $\mathcal{I}_{\mathcal{A}, \mathcal{A}'}$ the set of interface edges between them.

An aggregation of \mathcal{G} defines the subspace V_H of V consisting of “functions” taking constant value on every aggregate. This admits a multilevel hierarchy: solution of the variational problem $Au = f$ can be approximated by u_H from V_H which solves $(Au_H, v_H) = (f, v_H)$ for all $v_H \in V_H$. In this talk we assess the quality of an aggregation by measuring how well u_H approximates the solution u .

ASSESSING AGGREGATION QUALITY VIA A POSTERIORI ESTIMATION

We now give generalizations of two well known results that can be used in functional (hyper-circle) a posteriori estimates on graphs, or, in general Hilbert space settings. Let us set $\mathbf{W}(g) = \{\boldsymbol{\tau} \in \mathbf{W} \mid (\boldsymbol{\tau}, G\phi) = g(\phi), \forall \phi \in V\}$.

Lemma 1. [Prager-Synge [1]] Let u be the solution to $Au = f$, where A is a (graph) Laplacian. For any $\boldsymbol{\tau} \in \mathbf{W}(f)$ and any $v \in V$, the following identity holds.

$$\|u - v\|_A^2 + \|DGv - \boldsymbol{\tau}\|_{D^{-1}}^2 = \|DGv - \boldsymbol{\tau}\|_{D^{-1}}^2.$$

Lemma 2. [S. Repin [2]] Let u be the solution to $Au = f$ and λ be the smallest positive eigenvalue of A . Assume that $\boldsymbol{\phi} \in \mathbf{W}$ is arbitrary. Then for all $v \in V$:

$$\|u - v\|_A \leq \|DGv - \boldsymbol{\phi}\|_{D^{-1}} + \lambda^{-1} \|G^* \boldsymbol{\phi} + f\|.$$

If $v = u_H$, then we get the following error estimator

$$\|u - u_H\|_A \leq \eta(\boldsymbol{\phi}), \quad \eta(\boldsymbol{\phi}) = \|Gu_H - \boldsymbol{\phi}\| + C_P^{-1} \|G^* \boldsymbol{\phi} + f\|$$

To get a reliable lower bound of $\eta(\boldsymbol{\phi})$ we are free in the choice of $\boldsymbol{\phi} \in \mathbf{W}$, so we can minimize $\eta(\boldsymbol{\phi})$ with respect to $\boldsymbol{\phi}$. This could be time consuming (computing a global minimizer on \mathbf{W}), and we do this on a subspace \mathbf{W}_H . For each interface $\mathcal{I}_{\mathcal{A}, \mathcal{A}'}$, fix aggregate \mathcal{A} and define a basis function $\boldsymbol{\phi}_{\mathcal{I}} = Q_{\mathcal{I}} G \mathbf{1}_{\mathcal{A}}$, where $Q_{\mathcal{I}}$ is the l_2 projection onto \mathcal{I} . We then define $\mathbf{W}_H = \text{Span}_{\mathcal{I}} \{\boldsymbol{\phi}_{\mathcal{I}}\}$.

AGGREGATION RESHAPING ALGORITHM AND NUMERICAL EXAMPLES

We use the estimator $\eta(\boldsymbol{\phi})$ to devise an algorithm for forming aggregations adapted to the right-hand side. For given right-hand side f and any aggregation we denote the minimum of $\eta(\boldsymbol{\phi})$ over \mathbf{W}_H by $\eta(f)$. Then the estimator is localized as follows: Define

$$\tilde{\eta}_{\mathcal{A}} := \frac{1}{2} \sum_{\mathcal{A}'} \sum_{e \in \mathcal{I}_{\mathcal{A}, \mathcal{A}'}} \|Gu_H - \boldsymbol{\phi}\|_e^2 + \sum_{e \in \mathcal{E}_{\mathcal{A}}} \|Gu_H - \boldsymbol{\phi}\|_e^2 + C_P^{-2} \|G^* \boldsymbol{\phi} + f\|_{\mathcal{V}_{\mathcal{A}}}^2.$$

It can be shown that $\eta^2(f) \leq 2 \sum_{\mathcal{A}} \tilde{\eta}_{\mathcal{A}}$. Our reshaping algorithm then splits the aggregates on which $\tilde{\eta}_{\mathcal{A}}$ is large, with the aim to reduce the value of the estimator.

Algorithm 0.1 Reshaping of an aggregation

- 1: Given graph \mathcal{G} , aggregation $\{\mathcal{A}_k\}_{k=1}^{n_c}$
 - 2: (**Init**) Compute u_H and $\boldsymbol{\phi}$, minimizing $\eta(f, \mathcal{A})$
 - 3: (**Split**) Split all \mathcal{A}_k such that $\tilde{\eta}_{\mathcal{A}_k} > \frac{\sum_{i=1}^{n_c} \tilde{\eta}_{\mathcal{A}_i}}{n_c}$,
 - 4: stop if criterion is met (e.g. n_c larger than a threshold N), else go to step **Init**.
-

We perform experiment with reshaping starting from a coarse aggregation formed by matching. By matching we mean an algorithm that aggregates graphs by grouping two neighboring vertices (or aggregates) together at a time.

Let V_h and V_H be the subspaces of V obtained after k_0 and k_1 iterations of matching, respectively, $k_0 < k_1$ so that V_h is finer than V_H . We solve for u_h on

Aggregation	n_c	e_{ff}	$\ u_h - u\ _A / \ u\ _A$
$k_0 = 3$	1798	1.9465	0.8456
$k_1 = 7$ then reshape	742	1.1667	0.8223
$k_0 = 4$	837	1.7117	0.9020
$k_1 = 7$ then reshape	354	1.1532	0.8939
$k_0 = 5$	395	1.5754	0.9335
$k_1 = 7$ then reshape	250	1.1587	0.9195
$k_0 = 6$	190	1.4575	0.9586
$k_1 = 7$ then reshape	143	1.1468	0.9499

TABLE 1. Results for aggregations with and without reshaping

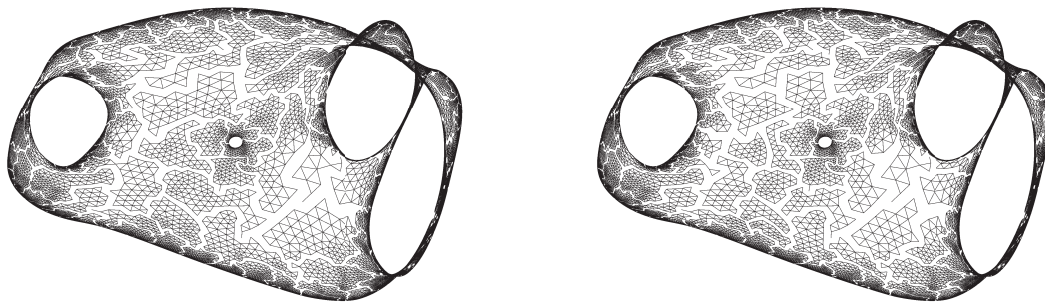


FIGURE 1. Adaptive aggregations. Left: $k_0 = 6$, $n_c = 190$; Right: $k_1 = 7$ with reshaping, $n_c = 129$. Graph `barth5` from University of Florida Sparse Matrix Collection:

<http://www.cise.ufl.edu/research/sparse/matrices/>

V_h for a smooth (global) f and compute the error $e_h = \|u - u_h\|_A$. Then the reshaping algorithm is performed on V_H , starting from the coarsest grid, and then the aggregates are split in exactly the same way they were formed in matching. We do this recursively until the error e_H on V_H becomes smaller than e_h .

The numerical results are shown in table 1. We can see that to achieve the same approximation error, reshaping significantly reduces the number of aggregates. Figure 1 plots the aggregations formed by matching ($k_0 = 6$) and by reshaping (started from $k_1 = 7$ with $n_c = 92$).

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Parallel multigrid reduction in time (MGRIT) with space-time adaptivity

ROBERT D. FALGOUT

(joint work with Veselin Dobrev, Tzanio Kolev, Matthieu Lecouvez, Ben O'Neill, Jacob Schroder, Ben Southworth, Ulrike Yang)

Since clock speeds are no longer increasing, time integration is becoming a sequential bottleneck. The multigrid reduction in time (MGRIT) algorithm is an approach for exploiting parallelism in the time dimension that is designed to build on existing codes and time integration techniques. The XBraid library is an open source implementation of MGRIT. One important technique used by current simulation codes is adaptivity in both space and time. In this talk, we discuss approaches taken in XBraid to support adaptivity by exploring several application problems that employ a combination of mesh refinement, mesh motion, and temporal refinement. For more details on MGRIT and XBraid, and their use in various application settings, see [1, 2, 3, 4, 5, 6, 7].

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(Ideas about) Adaptive FEM for problems with time-dependent domains

ALFRED SCHMIDT

(joint work with Carsten Niebuhr)

Due to thermomechanical distortions during a milling process, the shape of the produced workpiece is typically not correct. In order to estimate the shape error and as a prerequisite for an optimization of the process, a numerical model was

set up. It consists of a process model, giving heat flux and forces at the cutting boundary, and a workpiece model handling the material removal (giving the time-dependent domain) and a finite element model for thermomechanics on this time-dependent domain.

The system of equations for temperature θ and deformation u on the time-dependent domain $\Omega(t)$ is given by

$$\begin{aligned} \dot{\theta} - \operatorname{div}(\kappa \nabla \theta) &= 0 && \text{in } \Omega(t), \\ n \cdot \kappa \nabla \theta &= q && \text{on } \Gamma(t), \\ -\operatorname{div} \sigma(u) &= 0 && \text{in } \Omega(t), \\ n \cdot \sigma(u) &= g && \text{on } \Gamma_N(t), \\ u &= 0 && \text{on } \Gamma_D, \end{aligned}$$

where $\Gamma(t) = \partial\Omega(t)$ with subsets of clamped boundary Γ_D and mechanically free boundary $\Gamma_N(t)$. $q(x, t)$ denotes the heat flux into the material and $g(x, t)$ the external forces, both produced by the milling process. $\sigma(u)$ denotes the usual linear stress tensor. Let's assume here that the current domain $\Omega(t)$ is given. In the application, the shape of the domain is part of the unknowns, as the cutting tool path is typically prescribed (or subject to optimization) and workpiece deformation leads to incorrect material removal.

The interesting part of this model is the treatment of the time-dependent (shrinking) domain due to material removal. We present and discuss several approaches for handling this in a finite element method. In a finite element context, our approach uses a discrete approximation of the domain $\Omega(t_k)$ by the union of all elements of the triangulation \mathcal{T}_k , which intersect the current domain,

$$\Omega_h(t_k) := \{T \in \mathcal{T}_k : T \cap \Omega(t_k) \neq \emptyset\}.$$

This results in a quite coarse approximation of order $O(h)$, but is easy to implement as the approach doesn't need to cut mesh elements or move vertices to the current boundary $\Gamma(t_k)$. A local mesh refinement near the moving boundary is used for better approximation, see Figure 1 for a 2D sketch.

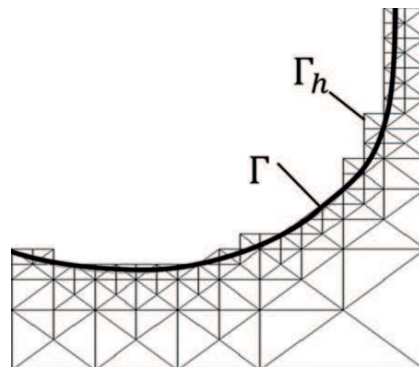


FIGURE 1. Approximation of the domain with continuous and discrete boundaries.

The Neumann boundary condition, namely

$$Q(v) := \int_{\Gamma(t)} q(x, t)v(x)dx$$

in the weak form with test function $v \in H^1(\Omega(t))$, has to be transferred to the discrete problem. The standard approach is to define a Neumann condition on the approximate boundary $\Gamma_h(t) = \partial\Omega_h(t)$,

$$Q_h(v_h) := \int_{\Gamma_h(t)} q_h(x, t)v_h(x)dx$$

where q_h is a modification of q which has to account for the different surface size of $\Gamma(t)$ and $\Gamma_h(t)$, in order to keep the total heat flux into the workpiece correct [3] (typically, the discrete boundary Γ_h consisting of mesh element boundaries is larger than a smooth given boundary Γ). The same is done for the Neumann forces in the elasticity equation. Using this approach together with a dixel model for computing the time-dependent domain and an appropriate process model for generating heat flux and forces from the path of the milling tool, we are able to simulate the thermal distortion of a workpiece during the milling process, see Figure 2, which compares well with experiments [2].

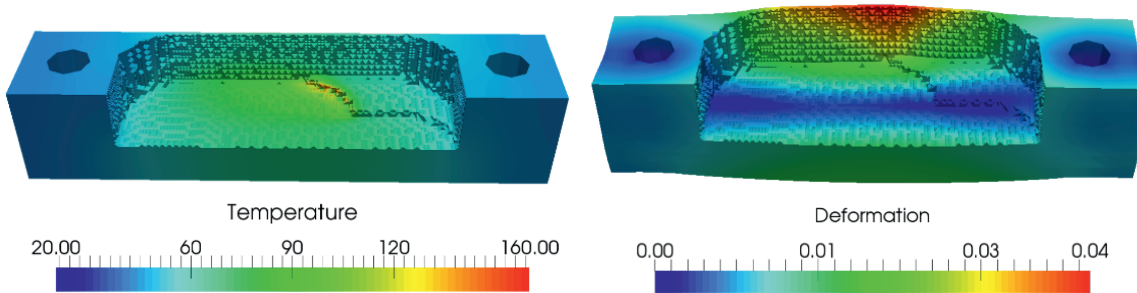


FIGURE 2. Simulation of the material removal and thermomechanics of a milling process: temperature and deformation during the process.

A special approach, namely interpreting the Neumann condition as an H^{-1} -functional, is discussed. Here, we use the correct functional even in the discrete case,

$$Q(v_h) := \int_{\Gamma(t)} q(x, t)v_h(x)dx.$$

In the situation described above, the discrete domain is always larger than the continuous domain, $\Gamma(t_k) \subset \bar{\Omega}_h(t_k)$, and the integral is well defined. Additionally, when $\Gamma(t_k)$ and q are given as piecewise (bi-) linear data, e.g., the integral can be evaluated exactly. Using the correct functional might lead to an appropriate error estimate with a-posteriori indicators.

The project is in cooperation with Jost Vehmeyer, Iwona Piotrowska, and Peter Maaß from ZeTeM, University of Bremen as well as Daniel Niederwestberg and

Berend Denkena from IFW, University of Hannover [1]. We gratefully acknowledge the support of DFG via Priority Program 1480 ‘Modeling, Simulation and Compensation of thermal effects for complex machining processes (CutSim)’.

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