Duality-Based Adaptive Finite Element Methods with Application to Time-Dependent Problems

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Doctoral Thesis No. 45, 2010
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To Miriam

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Abstract

To simulate real world problems modeled by differential equations, it is often not sufficient to consider and tackle a single equation. Rather, complex phenomena are modeled by several partial differential equations that are coupled to each other. For example, a heart beat involve electric activity, mechanics of the movement of the walls and valves, as well as blood flow – a true multiphysics problem. There may also be ordinary differential equations modeling the reactions on a cellular level, and these may act on a much finer scale in both space and time. Determining efficient and accurate simulation tools for such multiscalar multiphysics problems is a challenge.

The five scientific papers constituting this thesis investigate and present solutions to issues regarding accurate and efficient simulation using adaptive finite element methods. These include handling local accuracy through submodeling, analyzing error propagation in time-dependent multiphysics problems, developing efficient algorithms for adaptivity in time and space, and deriving error analysis for coupled PDE-ODE systems. In all these examples, the error is analyzed and controlled using the framework of dual-weighted residuals, and the spatial meshes are handled using octree based data structures. However, few realistic geometries fit such grid and to address this issue a discontinuous Galerkin Nitsche method is presented and analyzed.

Keywords finite element methods, dual-weighted residual method, multiphysics, a posteriori error estimation, adaptive algorithms, discontinuous Galerkin

This thesis consists of an introduction and the following five papers.

Paper I. M. Larson, F. Bengzon and A. Johansson: *Adaptive Submodeling for Linear Elasticity Problems with Multiscale Geometric Features*, LNCSE 44, pp. 169–180, Springer Verlag, 2005.

Paper II. F. Bengzon, A. Johansson, M. Larson and R. Söderlund: *Simulation of Multiphysics Problems Using Adaptive Finite Elements*, LNCS 4699, pp. 733–743, Springer Verlag, 2007.

Paper III. D. Estep, V. Carey, A. Johansson, M. Larson and S. Tavener: *Blockwise Adaptivity for Time Dependent Problems Based on Coarse Scale Adjoint Solutions*, accepted to SIAM Journal on Scientific Computing, 2010.

Paper IV. V. Carey, D. Estep, V. Ginting, A. Johansson, M. Larson and S. Tavener: *Adaptive Finite Element Solution of Coupled PDE-ODE Systems*, preprint, 2010.

Paper V. A. Johansson and M. Larson: *A Discontinuous Galerkin Nitsche Method for Elliptic Problems on Fictitious Domains*, preprint, 2010.

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I dedicate this thesis to Miriam Kjellgren. Let's have fun in California!

August Johansson
Umeå, May 2010

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Papers I-V

Chapter 1

Introduction

Many phenomena can be described by partial differential equations, or PDEs. For example, electromagnetic fields are described by the Maxwell equations, quantum physics problems involve the Schrödinger equation, incompressible gases and fluids are described by the Navier-Stokes equations, and stresses and deformations in a structure are given by the Cauchy-Navier equations, to name a few. Except for in special cases when the data of the problem is particularly easy, these equations are impossible to solve analytically by pen and paper. Numerical solutions by computer simulations is the only option.

The finite element method is a general method for solving PDEs and this thesis is on developing efficient and accurate finite element methods for problems with different geometric scales, and problems involving coupled physical phenomena. We also address how to efficiently handle time dependent problems. The solid mathematical basis of finite element methods makes it possible not only to simulate a physical problem modeled by one of the equations mentioned above, but also to systematically and rigorously simulate and analyze more complex phenomena, such as problems involving many PDEs that are coupled to each other. This is of course of major interest in real world problems. Just think of a heart beat. It involves electrical stimuli and conduction, chemical reactions in the cells, mechanics when the heart muscles contract and fluid flow when the blood is pumped. Such types of interconnected problems are called multiphysics problems.

Each of the individual physical phenomena in a multiphysics problem

may be described by a partial differential equation, and solving a single of these accurately and efficiently may be a challenge. When they are coupled together, the problem can be extraordinarily difficult. This is even more true if the features of the problem vary on several different scales in space and time, so called multiscale problems.

In addition to the systematic procedure of dealing with coupled problems such as multiphysics problems, the mathematical basis for finite elements also makes qualitative and quantitative error control possible. This is a crucial part of any numerical method, since a simulation seldom gives an exact solution. Nonetheless we want an accurate answer, preferably in limited time and to a specified accuracy. Although this claim may sound primitive and clear, several questions may arise:

- How can one estimate the error in a simulation without knowing the exact solution?
- What is meant by accurate? Are we interested in the correct value of the solution everywhere, or just in a few locations in time and space?
- How can one design a method that is efficient with respect to time consumption, computer resources and algorithmic complexity but at the same time result in an accurate simulation?

Such questions are addressed in this thesis and at least partial answers to all three of these are given.

1.1 Objectives

The primal objectives of the thesis are the following.

- Develop finite element methods for time-dependent and/or coupled problems, including deriving a duality-based posteriori error estimates and formulating adaptive methods for controlling the errors in both space and time.
- Develop and implement efficient algorithms for handling adaptivity in time and space. Particularly investigate the use of octree data structures and methods for handling complex geometries on such structures.

1.2 Main Results

1.2.1 Submodeling for Linear Elasticity

Submodeling is a procedure to improve a given coarse finite element solution in a certain region of interest, by solving a local problem on a finer mesh in this region. Paper I describes this technique for problems in linear elasticity and presents an adaptive algorithm for automatic selection of the size of the submodel and to be able to control the discretization errors on the fine and coarse meshes. The algorithm takes advantage of a goal-oriented posteriori error estimates derived using duality techniques, see for example Bangerth and Rannacher [2]. The procedure is illustrated in a three dimensional industrial problem.

1.2.2 A Posteriori Estimates for Multiphysics Problems

Paper II illustrates and extends an existing systematic methodology for analyzing the error in one-way coupled multiphysics problems (see Larson and Bengzon [21]). The procedure is particularly useful for connecting already existing specialized single physics solvers. The extension in Paper II allows for time dependent problems and is illustrated using a model for pressure-driven contaminant transport in porous media. Duality-based a posteriori error estimates are derived and used in an adaptive algorithm.

1.2.3 Blockwise Adaptivity: A Novel Method for Efficient Space-Time Adaptivity

Adaptivity and in particular dual-weighted residual based adaptivity for time-dependent problems can be computationally very costly if the spatial and temporal meshes are changed in each time step. Paper III presents a novel method to resolve this issue by using a sequence of fixed but non-uniform spatial meshes in time. The elements of this sequence are called blocks, why the method is named blockwise adaptivity. Goal-oriented posteriori analysis are used to formulate several strategies on how to select these blocks and still satisfy an overall accuracy in an output functional. The strategies are illustrated on different types of evolution PDEs in one and three dimensions.

1.2.4 A Posteriori Error Analysis for Coupled PDEs and ODEs

Paper IV demonstrates a posteriori error analysis for a coupled PDE-ODE problem using the framework of dual-weighted residuals. The error estimates derived include discretization errors as well as errors in the data passed to and from the PDE and ODEs. In addition, since the ODEs in certain application are defined on a much smaller temporal and spatial scale than what can be resolved by the finite element discretization for the PDE, the error terms include possible projection errors arising when feeding the global PDE solution unto the local ODEs. Recovery errors due to passing the local ODE solutions to the PDE are also included in this analysis. The method is illustrated on a realistic problem consisting of a semilinear PDE and a set of nonlinear ODEs modeling the electrical activity in the heart. The adaptive algorithm used is based on the method of blocks described in Paper III.

1.2.5 A discontinuous Galerkin Nitsche Method for Elliptic Problems on Fictitious Domains

The numerical examples presented in Papers II–IV are on trivial geometries which are partitioned using shape regular hexahedra. Although such meshes are efficiently handled using octree data structures (see for example Frisken and Perry [15]), their usefulness in real world problems is limited since only limited objects can be well represented. One approach to retain the advantage of such data structures but still have proper and general geometry approximation is to use discontinuous Galerkin method based on Nitsche's method, see [23]. This idea is not new, but Paper V presents a rigorous procedure to avoid numerical instabilities by associating certain elements on the boundary with elements lying in the interior (cf. Burman and Hansbo [4, 5]). The method is proved to have optimal convergence and is illustrated on a three dimensional problem.

1.3 Future Work

There are several natural directions to pursue when it comes to future work and these particularly regard to the technique of Paper V and heart simu-

lation applications. Foremost, it is natural to consider adaptive methods for this technique. Since the interactions between discontinuous Galerkin finite elements involve evaluating jumps and fluxes, analysis and implementation of *hp*-adaptivity as should be investigated, see the overview [9].

The method could also be used in problems with moving boundaries, and the use of a level set function as a boundary representation alleviates this (see Sethian [24]). Another extension is to consider time-dependent problems. This, combined with a moving boundary, would allow the study how the electrical activity in the heart governs the mechanical movement using a realistic geometry. Since many medications rely on blocking or opening the channels for ion transport through the cell membrane, a detailed model of the cellular activity would allow for possibilities to simulate the effect of medical treatment on the performance of the heart.

The method of dual-weighted residuals can also be applied to optimization problems, which also have useful in heart simulations. For example, one can consider the inverse problem of determining regions with low conductivity, that is, trying to locate heart infarctions, see Sundnes et. al. [26] and the references therein. This is a important problem, since such simulation techniques could aid physicians diagnose patients with the condition called left bundle block. Under such conditions, the electrocardiogram, which is the standard diagnostic tool, is of limited use.

Chapter 2

Finite Element Methods

The origin of the finite element method has two paths. One is the development by engineers in the 1950s, where complicated engineering designs were decomposed into smaller elements. Typically this technology was found in structural engineering, where larger structures were deassembled into simpler components such as beams and rods. These smaller components were then coupled together systematically to be able to compute the stresses and the strains of the whole system. The development of such techniques was not at all restricted to academia, but took place at large corporations such as Boeing as well.

The other path follows the mathematical theory of partial differential equations developed in the 19th century. The first numerical method used were finite difference methods in the early 20th century, but as early as 1923 Courant (see [10]) introduced the method of decomposing a problem into triangles on which a weak minimization problem could be formulated.

The mathematical and the engineering paths were in principle separated until the 60s when finite difference schemes were developed for problems in variational form. The name "finite elements" was introduced by Clough in 1960 [8]. For a pleasant survey of the history of finite element methods, see Zienkiewicz's personal presentation [29].

In the following sections the principal details of finite element methods will be presented, using two model problems: the Poisson equation and the Heat equation.

2.1 Two Model Problems

To illustrate the finite element method it is instructive to study one of the most basic PDEs, namely the Poisson equation. Although it is usually the first partial differential equations that one encounters when studying finite element methods, it is not only an academic problem but appears in various physical contexts in industry today. For example, the equation appear when the problem is to find a potential such as an electrostatical or gravitational potential $u = u(x)$ in some domain $\Omega \subset \mathbb{R}^d$, where d is the dimension. If the system is subject to a force $f = f(x)$, which involve a charge density in an electrostatic problem or a mass density in gravitation, the Poisson equation reads

$$-\Delta u = f, \tag{2.1}$$

where $\Delta = \sum_{i=1}^{d} \partial^2/\partial x_i^2$ is the Laplacian.

The Poisson equation also appears when looking for stationary solutions to one of the most basic time-dependent equations, namely the heat or diffusion equation,

$$\dot{u} - \Delta u = f, \tag{2.2}$$

where $\dot{u} = \partial u/\partial t$. This equation may describe the variation in heat, in which case $u = u(x,t)$ is the temperature and $f = f(x,t)$ is a heat source. It can also model diffusive processes such as the spreading of a chemical, in which case u is the concentration and f is again a source term. Usually one seeks solutions in a time interval $[0, T]$.

For the above problems to have a unique solution, it is necessary to state auxiliary conditions on how the solution behaves on the boundary $\partial\Omega$ of Ω. These so called boundary conditions are usually of two types:

1. Dirichlet boundary conditions, in which the function value itself is specified as $u = g_D$. These are also called essential boundary conditions.

2. Neumann boundary conditions, which specify the normal derivative, or the flux of the solution on the boundary by $n \cdot \nabla u = g_N$. Another name for Neumann boundary conditions are natural boundary conditions, since they appear in the integration by parts of the Laplacian. Here and below we let n denote the outward unit normal on $\partial\Omega$.

If the right hand sides in the Dirichlet and Neumann conditions are zero, they are referred to as homogeneous boundary conditions. For uniqueness of time-dependent problems it is necessary to impose an initial condition $u(x,0) = u_0(x)$ at the starting time.

The power of the finite element method is illuminated when presenting it in an abstract formulation. To this end we proceed with a section on weak or variational formulation of a PDE and continue with the finite element approximation.

2.2 Variational Formulation

The finite element method takes advantage of an abstract mathematical framework similar to calculus of variations, and finite element solutions can in fact be seen as energy minimizing solutions. To present this framework a few mathematical tools are needed, see for example Evans [14] for details.

Recall that a Hilbert space V is a linear function space equipped with an inner product $(\cdot,\cdot)_V : V \times V \to \mathbb{R}$ with corresponding norm $\|\cdot\|_V = (\cdot,\cdot)_V^{1/2}$. When working with finite element methods for equations of the above type, the most common Hilbert spaces are $L^2(\Omega)$, where

$$(v,w)_{L^2(\Omega)} = (v,w)_\Omega = \int_\Omega vw \; dx, \tag{2.3}$$

and $H^1(\Omega)$, where

$$(v,w)_{H^1(\Omega)} = (v,w)_\Omega + (\nabla v, \nabla w)_\Omega. \tag{2.4}$$

Furthermore, $H_0^1(\Omega)$ denote the subset of functions in $H^1(\Omega)$ that are zero on the boundary. For time dependent problems, the notation $L^2(I,X)$ is used to denote functions such that $\int_I \|v\|_X^2 \; dt < \infty$. Hilbert spaces are complete spaces and the derivatives should be actually be interpreted in a weak sense, but such a thorough presentation is beyond the scope here.

Now, let a be a bilinear form, that is, a mapping $V \times V \to \mathbb{R}$ that is linear in both of its arguments and let l be a linear form $V \to \mathbb{R}$. The variational form of the Poisson equation with homogeneous Dirichlet boundary conditions reads: find $u \in V = H_0^1(\Omega)$ such that

$$a(u,v) = l(v), \quad \forall v \in V, \tag{2.5}$$

where

$$a(u, v) = (\nabla u, \nabla v)_\Omega, \tag{2.6}$$

$$l(v) = (f, v)_\Omega. \tag{2.7}$$

The variational form is obtained by multiplying the PDE by a test function $v \in V$ and integrate by parts. It should be noted that there are two derivatives on u in the original equation, compared to only one in the bilinear form which reduces the smoothness requirements on the solution. This procedure is the same for all types of elliptic PDEs, for which the Poisson equation is the prototype problem.

For each equation and for each boundary condition one must choose appropriate spaces for finding u, called the trial space, and for v, called the test space. Here, the test and trial spaces are the same, but this is not the case for problems with both homogeneous and non-homogeneous boundary conditions, for example. Existence and uniqueness of solutions are assured by a theorem known as The Lax-Milgram Lemma if the forms are continuous and the bilinear form is coercive, see for example Ciarlet [7] or Brenner and Scott [3].

For the heat eqation with homogeneous Dirichlet boundary conditions the appropriate test and trial space is $W = L^2([0, T], H_0^1(\Omega))$. A weak formulation reads: find $u \in W$ such that

$$\int_0^T (\dot{u}, v) + a(u, v)\ dt = \int_0^T l(v)\ dt, \quad \forall v \in W. \tag{2.8}$$

The procedure for deriving the weak forms of these type of PDEs known as parabolic PDEs, is the same as for elliptic PDEs. The theory for proving existence and uniqueness is, however, a bit more elaborate. The interested reader is encouraged to study Evans [14] or Thomée [27].

2.3 Finite Element Discretizations

Given the variational formulation of the PDE of interest, the problem for finding the finite element solution is based on the same weak form, but using finite dimensional test and trial spaces. These are subspaces of V and here denoted by V_h. Similarly we have for time-dependent problems $W_h \subset W$.

Choosing a suitable finite element space can be a difficult task, but a good principle is to let the function space incorporate important physical features of the problem. On this function space a set of basis functions are needed. These are typically chosen to be piecewise polynomials since they are easy to work with, both in the analysis and in computer implementation.

To construct basis functions for the finite element spaces, the domain Ω (or space-time domain $[0,T] \times \Omega$) is usually partitioned into smaller subdomains, called elements. These elements, denoted by K, form a triangulation or a mesh $\mathcal{K}$ which approximate Ω (or $[0,T] \times \Omega$). Common shapes for the elements are triangles and quadrilaterals in two dimensions, or tetrahedra and hexahedra in three dimensions. The reasons for using such shapes are simplicity and generality, again both in the analysis and implementation. Creating discretizations for one-dimensional variables such as time is easier; for the time interval $[0,T]$ one can simply consider a partition $t_0 = 0 < t_1 < \cdots < t_N = T$ and form elements $I_n = (t_{n-1}, t_n]$, $n = 1, \ldots, N$.

It should be emphasized that these choices of rather primitive components in the discretization, using simple polygonal shapes as elements and polynomials for the basis, allow for efficient implementation as well as error control. This is due to the fact that errors are usually expressed in terms of the sizes of the elements and the order of the basis. To reduce the errors, one can thus split the elements or increase the order of the basis, either locally or globally. These are operations which are not trivial but, as shown in the results in this thesis, doable with good results.

Depending on the choices of finite element spaces V_h or W_h, one will obtain different finite element methods with different qualities. Nevertheless, the basic method can be understood by studying simple model problems as is done here.

A variety of finite elements are used in this thesis. Paper I uses linear and quadratic polynomial bases on tetrahedra, Papers II-V uses trilinear and triquadratic bases on hexahedral elements where Papers III and IV in addition use temporal bases up to order three. Paper V investigates the use of super elements composed of a hexahedra plus a smaller region using a discontinuous basis.

For introductory texts on finite elements, see Eriksson et. al. [12], Johnson [20] or Larsson and Thomée [22]. For a more mathematical pre-

sentation, see Ciarlet [7] or Brenner and Scott [3]. Finite element methods for parabolic problems are thoroughly investigated in Thomée [27].

2.4 The Poisson Equation

To illustrate the finite element method in detail we return to the first model problem. Let $u_h = u_h(x)$ denote the finite element approximation, and let test and trial spaces be $V_h \subset V$. Typically these are continuous piecewise polynomials, that is,

$$V_h = \{v \in C(\Omega) : v(x)|_K \in \mathbb{P}^p(K),\ \forall K \in \mathcal{K}\}, \tag{2.9}$$

where $\mathbb{P}^p$ is the space of polynomials of order p. The typical finite element method for (2.5) now reads: find $u_h \in V_h$ such that

$$a(u_h, v) = l(v), \quad \forall v \in V_h. \tag{2.10}$$

It is here possible to give a geometrical interpretation of the method. Since $V_h \subset V$, taking an arbitrary $v \in V_h$ in (2.5) and subtracting (2.10) gives what is called the Galerkin orthogonality,

$$a(u - u_h, v) = 0. \tag{2.11}$$

The approximate solution $u_h \in V_h$ can thus be seen as a projection of the true solution u onto V_h, or equivalently, that the error $u - u_h$ is orthogonal to the subspace V_h. Of course, the terms projection and orthogonal are with respect to the weak form used as represented by the bilinear form.

Determining u_h is now at least in principle easy. Let $\{\varphi_i\}_{i=1}^m$ be a basis of V_h, such that u_h may be written as

$$u_h(x) = \sum_{j=1}^{m} U_j \varphi_j(x). \tag{2.12}$$

Moreover, testing against all functions in V_h is equivalent to test against all functions in the basis. Thus, (2.10) is equivalent to finding the coefficients U_j, $j = 1, \ldots, m$, such that

$$\sum_{j=1}^{m} a(\varphi_j, \varphi_i) U_j = l(\varphi_i), \quad i = 1, \ldots, m, \tag{2.13}$$

since a is bilinear. This is an $m \times m$ linear system

$$AU = b, \tag{2.14}$$

where $A_{ij} = a(\varphi_j, \varphi_i)$, $b_i = l(\varphi_i)$ and $U = (U_1, \ldots, U_m)^T$. The matrix A with these particular components is for historical reasons called the stiffness matrix. The right hand side vector is called the load vector. Finding u_h thus reduces to solving a linear system. How easy or hard it may be to solve this linear system depend on the PDE as well as the approximation space V_h.

2.5 The Heat Equation

The finite element discretization procedure for parabolic equations is very similar to the one shown for elliptic equations. For the time dependent problem (2.8), the analogue to the above procedure is to have the basis functions be dependent on time. Another approach is to perform sequential semidiscretizations. Standard procedure is here to first discretize in space as above and let the coefficients be time dependent, then discretize in time.

Both when using a space-time basis or perform semidiscretizations, it is convenient and natural to introduce the temporal discretization of $[0, T]$ presented above: Create the partition $t_0 = 0 < t_1 < \cdots < t_N = T$ and denote each subinterval by $I_n = t_n - t_{n-1}$, $n = 1, \ldots, N$. The typical discrete space is

$$W_h^r = \{w(x,t) = \sum_{i=0}^{r} t^i v_i(x),\ v_i \in V_h,\ (x,t) \in I_n \times \Omega\}, \tag{2.15}$$

which says that on each space-time slab $S_n = I_n \times \Omega$, the basis is polynomial in both space, since $v_i \in V_h$, and time, since w is the sum over the canonical basis $1, t, \ldots, t^r$. Note that W_h^r allows for the basis to be discontinuous or continuous in time – see the remark in the end of this section regarding the discontinuous method.

The continuous finite element formulation is to find $u_h = u_h(x,t) \in W_h^r$ such that

$$\int_0^T (\dot{u}_h, v) + a(u_h, v)\ dt = \int_0^T l(v)\ dt, \quad \forall v \in W_h^{r-1}. \tag{2.16}$$

It is sufficient to test against functions in the lower order space W_h^{r-1} since the initial value is known and the solution is said to be continuous. Moreover, the formulation determines a Galerkin orthogonality similar to the Poisson problem, cf. (2.11).

In a spatially semidiscrete formulation one first expands u_h in the basis of V_h as in (2.12) and allow the coefficients U to be time dependent. This yields

$$\int_0^T \sum_{j=1}^{m} (\varphi_j, \varphi_i)\dot{U}_j + a(\varphi_j, \varphi_i)U_j \; dt = \int_0^T l(\varphi_i) \; dt, \quad i = 1, \ldots, m, \tag{2.17}$$

or in matrix form,

$$\int_0^T M\dot{U} + AU \; dt = \int_0^T b \; dt, \tag{2.18}$$

where $M_{ij} = (\varphi_j, \varphi_i)$ is called the mass matrix, and A, U and b are the same as for the Poisson problem (2.14). This is of course a vector valued equation, where the integrals are computed on each element in the vectors. Equation (2.18) can in principle be seen as a system of ordinary differential equation, and this approach gives the method of lines, see for example the early paper by Zafarullah [28].

From here it is possible to proceed in a few different ways. Standard procedure is to discretize the time derivative by for example finite differences. Another approach is to continue to use finite elements by seeking the solution in a finite dimensional space Q^r defined by

$$Q^r = \{w \in C^0([0,T]) : w \in [\mathbb{P}^r(I_n)]^m, \; n = 1, \ldots, N\}, \tag{2.19}$$

where C^0 is the space of continuous functions. The problem is thus to find $U \in Q^r$ such that

$$\int_0^T \langle M\dot{U}, w\rangle + \langle AU, w\rangle \; dt = \int_0^T \langle b, w\rangle \; dt, \quad \forall w \in Q^{r-1}, \tag{2.20}$$

where $\langle \cdot, \cdot \rangle$ is the vector-valued inner product on each component in $\mathbb{R}^m$, not the standard inner product.

Now we proceed as usual: Let $\{\vartheta^j\}_{j=1}^N$ be a vector-valued basis for Q^r and expand U in this basis as $U_k(t) = \sum_{j=1}^N U_k^j \vartheta_k^j(t)$, for each component

$k = 1, \ldots, m$. Given U^0, the coefficients U may be determined by evolving the following on each interval I_n, $n = 1, \ldots, N$ (with slight abuse of notation),

$$\int_{I_n} \langle M \sum_{j=1}^{N} U^j \dot{\vartheta}^j, w \rangle + \langle A \sum_{j=1}^{N} U^j \vartheta^j, w \rangle \; dt = \int_{I_n} \langle b, w \rangle \; dt, \quad \forall w \in Q^{r-1}. \tag{2.21}$$

Note the difference between this formulation and the one obtained for the Poisson problem: the test functions are not equal the basis functions of the trial space.

This slightly cumbersome but general procedure may produce familiar finite difference methods. For example, choosing $r = 1$, that is, a linear basis in time, gives the generalized Crank-Nicolson method

$$(M + \frac{k_n}{2} A) U^n = (M - \frac{k_n}{2} A) U^{n-1} + \int_{I_n} b \; dt, \tag{2.22}$$

where $k_n = t_n - t_{n-1}$. The standard Crank-Nicolson method is obtained using the trapezoidal rule on the integral in the right hand side.

Note that the each of the m components in U are discretized in the same space; having individual spaces, for example with a different temporal discretization or using basis functions of different order, allow for sophisticated adaptive methods.

Remark. Although W_h^r allows for discontinuous functions in time, this choice is incompatible with the variational form (2.16). One must then instead consider

$$\int_{I_n} (\dot{u}_h, v) + a(u_h, v) \; dt + ([u_h]_{n-1}, v^+) = \int_{I_n} l(v) \; dt, \quad \forall v \in W_h^q, \tag{2.23}$$

where $[\cdot]$ denotes the jump across adjacent time intervals. Given this variational formulation, it is possible to see that piecewise constant basis functions yield a generalized backward Euler method,

$$(M + k_n A) U^n = \int_{I_n} b \; dt. \tag{2.24}$$

The classical method is obtained using endpoint quadrature in the integral on the right hand side.

2.6 Different Finite Element Methods

It is important to note that both the variational form used in the finite element method and the solution spaces V_h and W_h^q may differ for the same PDE. Thus we may have different finite element methods for the same PDE, with different approximate solutions. These liberties has lead to a variety of different finite element methods.

For example, the family of methods known as Extended finite element methods, or XFEM, takes advantage of the liberty of enriching the solution space with discontinuous functions, see for example the papers from the Belytschko and co-workers [6]. Hughes et. al. have developed a method of using a certain family of smooth splines as basis functions. These splines, called NURBS, are used in computer aided design software and can thus represent the domain Ω very well. See the survey [18] for more details.

The freedom of choosing which weak form the finite element solution will fulfill is used in discontinuous Galerkin, or dG, methods. These methods are found to be useful from problems with highly localized gradients such as shocks. In a dG method the approximate solution is usually a piecewise polynomial on each element K and discontinuous across element faces E and therefore the weak forms will include jumps, denoted by $[\cdot]$, and averages, denoted by $\langle\cdot\rangle$, across the edges. For an extensive overview of dG methods, see the survey by Arnold et. al. [1] as well as Cockburn et. al. [9].

As an example, the weak form used in Paper V for the Poisson equation reads: Find $u_h \in \bigoplus_{K\in\mathcal{K}} \mathbb{P}^p(K)$ such that $a(u_h, v) = l(v)$, where

$$\begin{aligned} a(v,w) = &\sum_{K\in\mathcal{K}} (\nabla v, \nabla w)_K - \sum_{E\in\mathcal{E}} (\langle n\cdot\nabla v\rangle, [w])_E \\ &- \sum_{E\in\mathcal{E}} ([v], \langle n\cdot\nabla w\rangle)_E + \sum_{E\in\mathcal{E}} (\beta h_E^{-1}[v], [w])_E, \end{aligned} \tag{2.25}$$

$$l(v) = (f, v). \tag{2.26}$$

Here $\mathcal{E}$ is the set of edges, h_E denotes the size of an edge, and β is a penalty. Note that this weak formulation is equivalent to the continuous formulation (2.10) if a continuous basis is used.

The method was originally presented by Nitsche [23] as a way to weakly enforce Dirichlet boundary conditions and the method has been used extensively in discontinuous Galerkin settings, where it is also known as the

symmetric interior penalty method. Its use for handling boundaries and interfaces has been developed by Hansbo et. al. for immersed boundaries, as investigated in [16, 17], as well as to handle fictitious domains. However, if the boundary cuts through an element such that there is only a small fraction of the element inside the domain, the method is numerically unstable due to limited coupling of the outermost nodes. Some way of circumventing this is necessary and in Paper V this is done by associating each such element with a sufficiently large element. Other solutions are stabilization techniques, see Hansbo and Burman [4, 5].

Other techniques for handling immersed boundaries include the ESIC method by Sethian and Huh [19], where an exact construction is used to enhance the solution at the elements containing the interface. Extended finite element methods can also be applied to such problems, see for example [25].

Chapter 3

Duality-Based A Posteriori Error Estimates

As mentioned in the introduction, any numerical method is likely to produce errors. One advantage with using Finite Elements is the solid mathematical foundation which allows for systematic analysis of the errors involved.

Error estimates can generally be classified as either of a priori or of a posteriori type. The former give bounds on the errors in terms of the exact solution u and the global mesh size h and time step k, thus able to express the order of accuracy of the method. Typically, if a basis of order p is used in space and of order r in time, the error is bound by $\|e\| \leq C(h^{p+1} + k^{r+1})$. Note that the exact solution u solution is needed to evaluate the estimate, which is unknown.

A posteriori error analysis, on the other hand, give bounds on the error e using the computed solution u_h and the element mesh size h_K and time step k_n, making such estimates directly computable. The motivation for a posteriori analysis is twofold. One reason is to derive error estimates, or at least approximate error estimates, to be able to compute an approximation of the error in the computation. Another reason is to be able identify the elements that have a large contribution to the error thus suitable for adaptive algorithms, which are procedures for refining elements with large error contributions. To this end, the estimates should separate error contributions from different sources and express them in terms of adjustable parameters, such as h_K and k_n.

Furthermore, in real world problems one is usually interested in some functional of the solution, such as the lift on the wings when computing the air flow around an airplane, which means that not all of Ω is of equal importance. This kind of reasoning has driven the development of what is called goal-oriented error estimates. The basic idea is that if the spatial errors are large in a subregion (or possibly the entire domain), reducing the element sizes in this region will reduce the error. The selection of elements is determined using a posteriori estimates. It is also possible to reduce the error in such regions by changing to a basis of higher order. The former is called h-adaptivity, the latter p-adaptivity and a combination of the two is called hp-adaptivity. Similarly it is possible to control temporal errors.

Goal-oriented estimates are a posteriori error estimates where the error in a functional of the solutions is weighted with the solution to an auxiliary problem. This additional problem, called the dual or the adjoint problem, contains the sensitivity of the error with respect to the given goad functional. Therefore such estimates are also known as dual-weighted estimates.

The standard framework for deriving a posteriori error estimates is the dual-weighted residual method, which is reviewed in the next section. For a thorough review of such methods, see Bangerth and Rannacher [2] or Estep et. al. [13] (specifically for reaction-diffusion systems). For a general overview of using a posteriori estimates in adaptive computations, see for example the survey by Eriksson et. al. [11].

3.1 An Example from Linear Algebra

The principle of dual-weighted error estimates, can be illustrated using a problem from linear algebra. Let A be an invertible $n \times n$ matrix, let b be a given $n \times 1$ vector and consider the problem of finding u given by the linear system

$$Au = b. \tag{3.1}$$

However, if for some reason the only attainable solution is u_h, there is an error e given by

$$e = u - u_h, \tag{3.2}$$

and a residual r given by

$$r = b - Au_h. \tag{3.3}$$

Note that the error is unknown, but the residual is known why it is desirable to bound the error in terms of the residual. Before embarking on the analysis some notation is required.

Let $\langle \cdot, \cdot \rangle$ denote an inner product on $\mathbb{R}^n$ with corresponding norm $\|\cdot\|$, and let $\psi \in \mathbb{R}^n$. Now, $\langle \psi, e \rangle$ weigh different parts of the error differently. For example, let $\psi = (1, \ldots, 1)^T/n$ to obtain the average error or let $\psi = (1, 0, \ldots, 0)^T$ to obtain the error in the first entry of the approximate solution. In fact, recall that the Riesz Representation Theorem says that any linear functional of e can be identified by a particular ψ and an inner product. This is a key feature of goal-oriented error control. The procedure to derive the error estimate is as follows. First, consider the adjoint, or dual, problem of finding the $n \times 1$ vector ϕ such that

$$\psi = A^T \phi. \tag{3.4}$$

Multiplying the dual problem by e yields what is called an error representation formula, which expresses the error in the desired quantity as defined by ψ:

$$\begin{aligned} \langle e, \psi \rangle &= \langle e, A^T \phi \rangle && (3.5)\\ &= \langle Ae, \phi \rangle && (3.6)\\ &= \langle Au - Au_h, \phi \rangle && (3.7)\\ &= \langle b - Au_h, \phi \rangle && (3.8)\\ &= \langle r, \phi \rangle. && (3.9) \end{aligned}$$

This is an exact error representation formula if (3.4) is solved exactly. If not, it is possible to derive an error estimate using the Cauchy-Schwartz inequality, such that

$$|\langle e, \psi \rangle| \leq \|r\| \|\phi\|, \tag{3.10}$$

for which it is sufficient to know a bound on $\|\phi\|$ for example using an approximate solution ϕ_h.

This simple calculation illustrate the important feature of goal-oriented error estimates: The residual is weighted by an auxiliary function, the adjoint, such that different parts of the residual are more important than others.

3.2 A Posteriori Analysis for the Poisson Problem

In this section a dual-weighted a posteriori error estimate for the Poisson problem above will be derived, following the methodology presented in the previous section. Assume there is a quantity of interest given by the functional $m(u)$, define the adjoint problem of finding $\phi \in V$ by

$$m(v) = a(v, \phi), \quad \forall v \in V, \tag{3.11}$$

where a is the bilinear form (2.6). Note that since $\phi \in V$, it is in contrast to the adjoint solution to in the linear algebra example, not computable. If m is nonlinear, one approximates with the linearized quantity. This is explained further in the Remark at the end of this section.

Given the goal quantity $m(u)$ it is essential to control the error $m(u) - m(u_h) = m(e)$. Since $e \in V$, let $v = e$ in the adjoint problem (3.11) to obtain the error representation formula

$$\begin{aligned} m(e) &= a(e, \phi) && (3.12)\\ &= a(u - u_h, \phi) && (3.13)\\ &= l(\phi) - a(u_h, \phi) && (3.14)\\ &= (R(u_h), \phi), && (3.15) \end{aligned}$$

where $R(u_h)$ is the weak residual such that $(R(u_h), v) = l(v) - a(u_h, v)$, for all $v \in V$. Note that $R(u_h)$ is a computable quantity. This is the error representation formula for the Poisson problem, with the dilemma that ϕ is not attainable. Unfortunately, it is not satisfactory to approximate ϕ with a $\phi_h \in V_h$, since $a(u - u_h, \phi_h) = 0$ according to the Galerkin orthogonality (2.11). The solution is to find an approximation to ϕ in a richer space than V_h. For example, if V_h contains linear functions one could seek ϕ_h in a space of quadratic functions and thus obtain an approximate error representation formula. One can also use the orthogonality to derive an error bound. Indeed, for any function $v \in V_h$,

$$m(e) = a(u - u_h, \phi - v). \tag{3.16}$$

A suitable choice of v is the interpolant of ϕ, denoted by $\pi\phi$. This yields

$$\begin{aligned} m(e) &= a(u - u_h, \phi - \pi\phi) && (3.17)\\ &= (R(u_h), \phi - \pi\phi). && (3.18) \end{aligned}$$

The reason for this choice is that interpolation theory can be used to bound $\phi - \pi\phi$ in appropriate norms. It can be shown that $|m(e)| \leq Ch^{p+1}$, see e.g. Bangerth and Rannacher [2].

Approximating ϕ with ϕ_h in a richer space than V_h, one can deduce the approximate error representation formula by using a sum over elements K in the triangulation $\mathcal{K}$ as

$$|m(e)| \approx \Big| \sum_{K \in \mathcal{K}} (R_K(u_h), \phi_h - \pi\phi_h) \Big|, \tag{3.19}$$

where $R_K(u_h)$ is the weak element residual

$$(R_K(u_h), v)_K = (f - \Delta u_h, v)_K + (\frac{1}{2}[n \cdot \nabla u_h], v)_{\partial K \setminus \partial\Omega}. \tag{3.20}$$

Here, the bracket $[n \cdot \nabla u_h]$ denote the jump of the normal derivative of u_h across neighboring elements. The factor $1/2$ is chosen to balance the boundary contributions equally over the neighboring elements. Note that using a linear basis, $\Delta u_h = 0$, and using higher order bases, $[n \cdot \nabla u_h] = 0$. The formula (3.19) is only approximate, since the approximate solutions ϕ_h is used. However, this error is negligible compared to the residual and the weight.

From the result (3.19) it is intuitive that $m(e)$ may be small, since it is likely that both the residual can be made small and that the weight $\phi_h - \pi\phi_h$ can be made small through mesh refinement.

Remark. If $m(\cdot)$ is nonlinear one usually linearizes around a linear combination of the true and approximate solution to form $m'(\cdot)$, where

$$m'(v) = \int_0^1 \frac{\partial m}{\partial u}(us + u_h(1-s))\ ds\ v. \tag{3.21}$$

The chain rule now gives

$$m'(e) = \int_0^1 \frac{\partial m}{\partial u}(us + u_h(1-s))\ ds\ e \tag{3.22}$$

$$= \int_0^1 \frac{\partial m}{\partial s}(us + u_h(1-s))\ ds \tag{3.23}$$

$$= m(u) - m(u_h). \tag{3.24}$$

This linearized functional is used as goal functional in (3.11).

For a general possibly nonlinear elliptic problem $a(u, v) = l(v)$ the linearized bilinear form a' must be used when forming the adjoint problem. The linearization is similar to the one in (3.21) and the calculation (3.12) – (3.15) still holds, since $a'(e, v) = a(u, v) - a(u_h, v)$.

Choosing ψ to be approximately the delta distribution gives the error in a small region. Similarly, an approximate dipole gives the derivative of the error in a small region. If $\psi = e/\|e\|$ the L^2 error is obtained. This is mostly of theoretical interest, since e is unknown. Similarly, choosing ψ to be the residual gives the error in the energy norm.

If it is found that there is a certain region that contribute significantly to the error in the goal quantity, it might be desirable to be able to consider this region separately. One procedure for doing this is called submodeling and is investigated in Paper I.

3.3 A Posteriori Analysis for the Heat Equation

A posteriori estimation for the heat equation follows the same path as just shown. Assuming that the error is to be controlled in the functional $m(e)$ over time, the adjoint problem reads: find $\phi \in W$ such that

$$\int_0^T m(v)\ dt = \int_0^T (v, -\dot{\phi}) + a(v, \phi)\ dt, \quad \forall v \in W. \tag{3.25}$$

Note that the adjoint problem is solved backwards in time. If the error at the end time is of interest, one can additionally use the final condition $\phi(T) = \psi$. Similarly to the procedure for the Poisson problem, we let $v = e$ and integrate by parts to obtain

$$\int_0^T m(e)\ dt = \int_0^T (e, -\dot{\phi}) + a(e, \phi)\ dt \tag{3.26}$$

$$= \int_0^T (\dot{e}, \phi) + a(e, \phi)\ dt - (e(T), \phi(T)) + (e(0), \phi(0)), \tag{3.27}$$

assuming e is continuous. Since the adjoint problem is exact it is reasonable to assume that there is no error in the initial data to the adjoint problem, giving $(e(T), \phi(T)) = 0$.

Before deriving the error representation formula it is necessary to introduce spatial and temporal projection operators

$$P : L^2(\Omega) \to V_h, \tag{3.28}$$

$$\pi_n : L^2(I_n) \to \mathbb{P}^q(I_n), \tag{3.29}$$

such that $P\pi_n = \pi_n P : L^2(I_n \times \Omega) \to W_h^q$. Since the exact solution u fulfills the equation and using $e(0) = (I - P)u_0$, the error representation formula reads

$$\int_0^T m(e)\ dt = \int_0^T (R(u_h), \phi)\ dt + ((I - P)u_0, \phi(0)) \tag{3.30}$$

$$= \int_0^T (R(u_h), \phi - \pi_n P\phi)\ dt + ((I - P)u_0, \phi(0)), \tag{3.31}$$

where $(R(u_h), v) = l(v) - (\dot{u}_h, v) - a(u_h, v)$ is the weak residual. The Galerkin orthogonality (2.16) is used to subtract the interpolant $\pi_n P\phi \in W_h^q$.

As for the Poisson problem, ϕ is approximated by ϕ_h in a richer space than W_h^q, for example $W_{h/2}^q$ or W_h^{q+1}. Writing the integrals as sums over the elements in space and time one obtains the following approximate error representation formula

$$\Big| \int_0^T m(e)\ dt \Big| \approx \Big| ((I - P)u_0, \phi(0)) + \sum_{n=1}^{N} \sum_{K \in \mathcal{K}} \int_{I_n} R_K(u_h), \phi_h - \pi\phi_h)_K\ dt \Big|, \tag{3.32}$$

where

$$(R_K(u_h), v)_K = (f - u_h - \Delta u_h, v)_K + (\frac{1}{2}[n \cdot \nabla u_h], v)_{\partial K \setminus \partial\Omega}, \tag{3.33}$$

is the weak element residual.

For a posteriori error estimates to be useful it is desirable to isolate error contributions from different sources and express them in terms of adjustable parameters. Papers III and IV in this thesis are heavily dependent on efficient space-time adaptivity, why separate error estimates for the spatial and temporal error are needed. To illustrate a procedure for

deriving such error estimates recall the true error representation formula (3.31) and write

$$\phi - \pi_n P\phi = \phi - P\phi + P\phi - \pi_n P\phi. \tag{3.34}$$

The result reads

$$\int_0^T m(e)\ dt = ((I-P)u_0, \phi(0)) \tag{3.35}$$

$$+ \int_{I_n} (R(u_h), \phi - P\phi)\ dt \tag{3.36}$$

$$+ \int_{I_n} (R(u_h), P\phi - \pi_n P\phi)\ dt \tag{3.37}$$

$$= I + II + III. \tag{3.38}$$

The error in initial data I

$$I = ((I-P)u_0, \phi(0)) \tag{3.39}$$

is computable and need no further analysis. Decomposing II as a sum over $\mathcal{K}$ and integrate by parts in space yields similarly to the Poisson problem

$$II = \sum_{K\in\mathcal{K}} \int_{I_n} (R_K^x(u_h), \phi - P\phi)\ dt, \tag{3.40}$$

where $R_K^x(u_h)$ is the weak spatial element residual

$$(R_K^x(u_h), v) = (f - \dot{u}_h + \Delta u_h, v)_K - (\frac{1}{2}[n\cdot\nabla u_h], v)_{\partial K\setminus\partial\Omega}. \tag{3.41}$$

Term III is similar to II,

$$III = \int_{I_n} (R^t(u_h), (I-\pi_n)P\phi)\ dt, \tag{3.42}$$

where

$$(R^t(u_h), v) = (f - \dot{u}_h + \Delta u_h, v). \tag{3.43}$$

Since $P\phi \in V_h$, this can be seen as an algebraic error in a semidiscrete method, i.e. corresponding to (2.18).

3.4 Error Indicators

As mentioned in the introduction to this chapter, one motivation for a posteriori estimates is to identify elements with a large contribution to the error. This is done by deriving quantities defined on the elements called element indicators which should depend on parameters that are easily adjustable in a computation, such as the size of the elements h_K or the length of the time intervals k_n.

Returning to the Poisson model problem and the approximate error representation formula (3.19), one example of an element indicator η_K is to simply let

$$\eta_K = |(R_K(u_h), \phi_h - \pi\phi_h)_K|. \tag{3.44}$$

If one does not want to compute ϕ_h in a richer space and subtract the interpolant, it is possible to use the Cauchy-Schwartz inequality and then bound $\|\phi - \pi\phi\|_K$ using interpolation estimates, see for example Johnson [20] or Brenner and Scott [3]. If one does not want to compute ϕ_h at all, one must show that it is bounded and use the same procedure. This will of coarse give a coarser error indicator, and it will not be "goal-oriented".

For the heat equation problem it is desirable to have one indicator for the spatial error and one indicator for the temporal error, to be able to control these errors separately. Fortunately, this is precisely what is done in the decomposition of the error in (3.38), where we can conclude the following.

- Term I (3.39) contributes to the spatial error – it is independent of time and the error in the projection can be reduced by decreasing the mesh size.
- Term II (3.40) can primarily be seen as a term contributing to the spatial error. The term is similar to (3.19) and thus the suitable indicator is similar to (3.44).
- Term III (3.42) is not explicitly dependent on the spatial mesh parameter, why this is set to be a temporal error indicator.

Consequently, spatial and temporal error indicators η_K and η_n for the

Heat equation can be defined as

$$\eta_K = \Big| \int_{I_n} (R_K^x(u_h), \phi_h - P\phi_h)\ dt \Big|, \tag{3.45}$$

$$\eta_n = \Big| \int_{I_n} (R^t(u_h), (I - \pi_n)\pi_n P\phi)\ dt \Big|, \tag{3.46}$$

where $R_h(u_h)$ is defined in (3.41) and $R_k(u_h)$ is defined in (3.43). As for the error indicator for the Poisson problem (3.44), there are various ways for simplifying these indicators.

3.5 Adaptive Algorithms

From the discussion in the introduction to this thesis, the typical objective of a simulation is to satisfy $|m(e)| < \text{TOL}$. Using a posteriori error estimates, the previous section show that it is possible to derive error indicators that are computable and give a bound on the errors on each element. An element error indicator η may approximate the error well, such that $|m(e)| \approx \sum \eta$, but whether or not this is necessary depend on the problem. It may be sufficient for the indicator to just give approximate information on where the error is large, which motivates the use of coarse approximations of the adjoint solution ϕ.

The prime use of error indicators are for identifying elements with large error contributions. To be able to refine such elements, a general h-adaptive algorithm for handling spatial errors is presented in Algorithm 1. Temporal errors can be handled analogously, as well as adaptivity with respect to the basis.

Here, LTOL is a local tolerance which may be determined in several ways. For example, using the Principle of Equidistribution which says that each element should contribute equally to the error, $\text{LTOL} \approx \text{TOL}/|\mathcal{K}_h|$, where $|\mathcal{K}_h|$ is the cardinality of $\mathcal{K}_h$.

The algorithm presented is the typical compute – estimate – mark – refine strategy commonly used, and this is the method used in Papers I and II. This method can indeed be used to control the error tolerance, but this is not addressed in those papers.

In Paper III a novel adaptive procedure for time dependent problems is presented using the concept of blocks. In each block, the spatial mesh is

Algorithm 1 Adaptive Finite Element Method

```
1: Choose an initial triangulation $\mathcal{K}_h$ and a tolerance TOL.
2: while $|m(e)| <$ TOL do
3:     Compute a solution $u_h$ to the primal problem.
4:     Compute a solution $\phi_h$ to the adjoint problem.
5:     Compute an estimate of $|m(e)|$.
6:     if $|m(e)| >$ TOL then
7:         Refine all elements with $\eta \geq$ LTOL.
8:     end if
9: end while
```

fixed but non-uniform and each block is defined on a certain time interval with a possibly non-uniform partition. This method is used in Paper IV computationally expensive coupled nonlinear PDE-ODE system.

Chapter 4

Summary of Papers

I. Adaptive Submodeling for Linear Elasticity Problems with Multiscale Geometric Features

Submodeling is a procedure for local enhancement of the resolution of a coarse global finite element solution by solving a local problem on a subdomain containing an area of particular interest. We focus on linear elasticity and computation of local stress levels determined by the local geometry of the domain. We derive a posteriori error estimates for the submodeling procedure using duality techniques. Based on these estimates we propose an adaptive procedure for automatic choice of the resolution and size of the submodel. The procedure is illustrated for problems of industrial interest.

II. Simulation of Multiphysics Problems Using Adaptive Finite Elements

Real world applications often involve several types of physics. In practice, one often solves such multiphysics problems by using already existing single physics solvers. To satisfy an overall accuracy, it is critical to understand how accurate the individual single physics solution must be. In this paper we present a framework for a posteriori error estimation of multiphysics problems and derive an algorithm for estimating the total error. We illustrate the technique by solving a coupled flow and transport problem with application in porous media flow.

III. Blockwise Adaptivity for Time Dependent Problems Based on Coarse Scale Adjoint Solutions

We describe and test an adaptive algorithm for evolution problems that employs a sequence of "blocks" consisting of fixed, though non-uniform, space meshes. This approach offers the advantages of adaptive mesh refinement but with reduced overhead costs associated with load balancing, re-meshing, matrix reassembly, and the solution of adjoint problems used to estimate discretization error and the effects of mesh changes. A major issue with a block-adaptive approach is determining block discretizations from coarse scale solution information that achieve the desired accuracy. We describe several strategies to achieve this goal using adjoint-based a posteriori error estimates and we demonstrate the behavior of the proposed algorithms as well as several technical issues in a set of examples.

IV. Adaptive Finite Element Solution of Coupled PDE-ODE Systems

We consider an implicit/explicit method for solving a semilinear parabolic partial differential equation (PDE) coupled to a set of nonlinear ordinary differential equations (ODEs). More specifically the PDE of interest is the heat equation where the right hand side couple with the ODEs. For this system, a posteriori error estimates are derived using the method of dual-weighted residuals giving indicators useful for constructing adaptive algorithms.

We distinguish the errors in time and space for the PDE separated from those from the ODEs and include errors due to transferring the solutions between the equations. In addition, since the ODEs in many applications are defined on a much smaller spatial scale than what can be resolved by the finite element discretization for the PDE, the error terms include possible projection errors arising when transferring the global PDE solution onto the local ODEs. Recovery errors due to passing the local ODE solutions to the PDE are also included in this analysis.

The method is illustrated on a realistic problem consisting of a semilinear PDE and a set of nonlinear ODEs modeling the electrical activity in the heart. The method is computationally expensive, why an adaptive algorithm using blocks is used.

V. A Discontinuous Galerkin Nitsche Method for Elliptic Problems on Fictitious Domains

We present a discontinuous Galerkin method, based on the classical method of Nitsche, for elliptic problems with an immersed boundary representation on a structured grid. In such methods very small elements typically occur at the boundary leading to breakdown of the discrete coercivity as well as numerical instabilities. In this work we propose a method that avoids using very small elements on the boundary by associating them to a neighboring element with a sufficiently large intersection with the domain. This construction allows us to prove the crucial inverse inequality that leads to a coercive bilinear form and as a consequence we obtain optimal order a priori error estimates. We also discuss the implementation of the method and present a numerical example in three dimensions.

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