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Stable and High-Order Finite Difference Methods for Multiphysics Flow Problems

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Abstract
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Partial differential equations (PDEs) are used to model various phenomena in nature and society, ranging from the motion of fluids and electromagnetic waves to the stock market and traffic jams. There are many methods for numerically approximating solutions to PDEs. Some of the most commonly used ones are the finite volume method, the finite element method, and the finite difference method. All methods have their strengths and weaknesses, and it is the problem at hand that determines which method that is suitable. In this thesis, we focus on the finite difference method which is conceptually easy to understand, has high-order accuracy, and can be efficiently implemented in computer software.

We use the finite difference method on summation-by-parts (SBP) form, together with a weak implementation of the boundary conditions called the simultaneous approximation term (SAT). Together, SBP and SAT provide a technique for overcoming most of the drawbacks of the finite difference method. The SBP-SAT technique can be used to derive energy stable schemes for any linearly well-posed initial boundary value problem. The stability is not restricted by the order of accuracy, as long as the numerical scheme can be written in SBP form. The weak boundary conditions can be extended to interfaces which are used either in domain decomposition for geometric flexibility, or for coupling of different physics models.

The contributions in this thesis are twofold. The first part, papers I-IV, develops stable boundary and interface procedures for computational fluid dynamics problems, in particular for problems related to the Navier-Stokes equations and conjugate heat transfer. The second part, papers V-VI, utilizes duality to construct numerical schemes which are not only energy stable, but also dual consistent. Dual consistency alone ensures superconvergence of linear integral functionals from the solutions of SBP-SAT discretizations. By simultaneously considering well-posedness of the primal and dual problems, new advanced boundary conditions can be derived. The new duality based boundary conditions are imposed by SATs, which by construction of the continuous boundary conditions ensure energy stability, dual consistency, and functional superconvergence of the SBP-SAT schemes.

Keywords: Summation-by-parts, Simultaneous Approximation Term, Stability, High-order accuracy, Finite difference methods, Dual consistency

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List of papers

This thesis is based on the following papers, which are referred to in the text by their Roman numerals.

I J. Lindström and J. Nordström. A stable and high-order accurate conjugate heat transfer problem. *Journal of Computational Physics, 229(14):5440–5456, 2010.*

II J. Berg and J. Nordström. Spectral analysis of the continuous and discretized heat and advection equation on single and multiple domains. *Applied Numerical Mathematics, 62(11):1620–1638, 2012.*

III J. Berg and J. Nordström. Stable Robin solid wall boundary conditions for the Navier–Stokes equations. *Journal of Computational Physics, 230(19):7519–7532, 2011.*

IV J. Nordström and J. Berg. Conjugate heat transfer for the unsteady compressible Navier–Stokes equations using a multi-block coupling. *Accepted for publication in Computers & Fluids, 2012.*

V J. Berg and J. Nordström. Superconvergent functional output for time-dependent problems using finite differences on summation-by-parts form. *Journal of Computational Physics, 231(20):6846–6860, 2012.*

VI J. Berg and J. Nordström. On the impact of boundary conditions on dual consistent finite difference discretizations. *Accepted for publication in Journal of Computational Physics, 2012.*

Contents

1. Introduction

Many problems in the natural sciences can be described in the language of mathematics as systems of partial differential equations (PDEs). A system of PDEs typically describes the time-evolution of physical quantities such as velocity, momentum, and energy in a coupled manner. There are no general methods to compute analytical solutions to PDEs, and even when there are analytical solutions available, they are often not suitable for practical applications due to their complexity. Numerical methods for solving the PDEs are therefore the preferred and often only choice.

The increase in computing power over the past decades has helped to establish numerical simulations as the third cornerstone of science, alongside theoretical analysis and practical experiments. As the usage of computers grow, the algorithms which produce the numerical results become increasingly important. In particular for solving PDEs, there is a multitude of available methods. Each of them have their strengths and weaknesses, and the problem at hand determines which method that is suitable.

In this thesis, the problems under consideration usually appear in computational fluid dynamics (CFD) applications. The typical and most general example is the compressible Navier–Stokes equations which describe the motion of a compressible fluid. The Navier–Stokes equations provide a challenge for both mathematicians and numerical analysts. From a mathematical point of view, it has not yet been proven that a global smooth solution exists in three space dimensions. From a numerical point of view, the treatment of boundary conditions and high complexity make the construction of numerical schemes highly non-trivial.

It is common in CFD to derive numerical methods for model problems which are subsequently applied to more complicated equations. Model problems are constructed so that the main mathematical properties of the real problem are preserved, but the analysis is simplified. Also, when implementing the solution algorithms for a model problem, flaws in the algorithms are not hidden by the algebraic complexity of the equations to be solved.

Whatever numerical method used to solve PDEs, the following requirements have to be satisfied;

1. Consistency
2. Stability
3. Efficiency

By the famous theorem of Lax and Richtmeyer [26], the solution of a linear PDE given by a numerical method converges to the solution of the PDE if,

and only if, the method is consistent and stable. All schemes which are used in practice are consistent by construction. Far from all schemes are, however, stable. That is what brings us to the main topic of this thesis—the construction of stable and high-order accurate numerical schemes for solving time-dependent partial differential equations.

2. The summation-by-parts technique

A finite difference method for solving differential equations is constructed by approximating the derivatives in discrete points as weighted sums of solution values in neighboring points. Recall the mathematical definition of the first derivative;

$$u'(x) = \lim_{h \to 0} \frac{u(x+h) - u(x)}{h}. \tag{2.1}$$

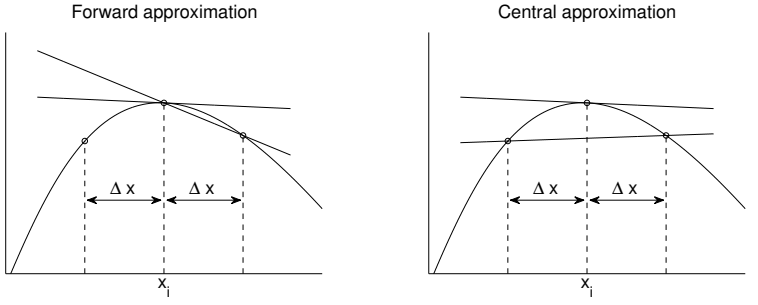
A computer has finite precision and hence h in (2.1) can not be made arbitrarily small. Instead, a computational grid is introduced where $h = \Delta x > \delta > 0$ and the first derivative at the point $x = x_i$ in (2.1) becomes approximated as

$$u'(x_i) \approx \frac{u(x_i + \Delta x) - u(x_i)}{\Delta x}. \tag{2.2}$$

In (2.2), only one neighbor-point is used. More points can be included to obtain more accurate approximations of the first derivative. For example the central approximation, where two neighbor-points are used, given by

$$u'(x_i) \approx \frac{u(x_i + \Delta x) - u(x_i - \Delta x)}{2\Delta x}. \tag{2.3}$$

The geometric interpretations of (2.2) and (2.3) can be seen in Figure 2.1.



(a) Forward difference using one neighbor-point

(b) Central difference using two neighbor-points

Figure 2.1. Geometric interpretation of first derivative approximation using forward and central differences

We say that (2.3) is second-order accurate since substituting the Taylor series expansion of $u(x)$ around $x = x_i$ gives

$$\frac{u(x_i+\Delta x)-u(x_i-\Delta x)}{2\Delta x} = u'(x_i) + \frac{\Delta x^2}{6}u^{(3)}(\xi) + \ldots,$$

where $x_i - \Delta x \leq \xi \leq x_i + \Delta x$. Thus if the third derivative of u is sufficiently smooth, the error term will behave as Δx^2 and tend to zero as $\Delta x \to 0$.

For Cauchy problems, the stability criteria for a given numerical scheme can be analyzed with von Neumann analysis. For an initial boundary value problem (IBVP), however, the formula (2.3) reveals difficulties. For example, if the point $x_i = x_0$ is a boundary point, then $x_0 - \Delta x$ is not included in the discretization and special care has to be taken.

The difficulties at the boundaries for IBVPs using finite difference methods is what gave birth to the summation-by-parts (SBP) form [23, 24]. We say that;

Definition 2.1. A finite difference matrix D_1 is an SBP operator for the first derivative if

$$\begin{aligned} D_1 &= P^{-1}Q, \\ Q+Q^T &= E_N - E_0 = \text{diag}[0,\ldots,0,1] - \text{diag}[1,0,\ldots,0], \end{aligned}$$

and the matrix P defines an inner product and norm by

$$(u_h, v_h)_h = u_h^T P v_h, \quad ||u_h||^2 = u_h^T P u_h,$$

for any discrete grid functions u_h, v_h.

Given these definitions, we have

$$(u_h, D_1 v_h)_h = u_h^T (E_N - E_0) v_h - (D_1 u_h, v_h)_h,$$

which mimics integration by parts in the continuous sense and motivates the SBP terminology. Essentially, an SBP operator is a central finite difference operator in the interior while the boundaries have been modified so that the operator is one-sided. For example, the second-order accurate operator is given by

$$D_1 = P^{-1}Q = \frac{1}{2\Delta x}\begin{bmatrix} -2 & 2 & 0 & 0 & \ldots & 0 \\ -1 & 0 & 1 & 0 & \ldots & 0 \\ 0 & -1 & 0 & 1 & \ldots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \ldots & 0 & -1 & 0 & 1 \\ 0 & \ldots & 0 & 0 & -2 & 2 \end{bmatrix},$$

where

$$P = \Delta x \begin{bmatrix} \frac{1}{2} & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & \dots & 0 & 1 & 0 \\ 0 & \dots & 0 & 0 & \frac{1}{2} \end{bmatrix}, \quad Q = \frac{1}{2} \begin{bmatrix} -1 & 1 & 0 & \dots & 0 \\ -1 & 0 & 1 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & -1 & 0 & 1 \\ 0 & \dots & 0 & -1 & 1 \end{bmatrix}.$$

There are SBP operators for the first derivative with interior order of accuracy $2p$ for $p = 1,2,3,4$. The global accuracy depends on the choice of the norm matrix P. With the requirement of P being diagonal, the order of accuracy at the boundaries needs to be reduced to p. The global order of accuracy then becomes $p+1$. There are also block-diagonal matrices which give $2p$-order global accuracy [46]. While a diagonal P gives less accuracy, it has more flexibility. For example, a diagonal norm is required to derive energy estimates under curvilinear coordinate transforms since P has to commute with the (diagonal) Jacobian matrix of the coordinate transform [37, 48]. In this thesis, a diagonal matrix P has been consistently used.

Once an energy estimate has been derived, a higher order accurate solution can be obtained by simply replacing the difference operator with one of higher order.

SBP operators can also be used to approximate the second derivative. The most direct way is to apply the first derivative twice, $D_2 = D_1 D_1$, which results in a wide difference stencil. The order of accuracy is the same as for the first derivative. A compact stencil can be obtained by considering a second derivative operator of the form

$$D_2 = P^{-1}(-A + (E_N - E_0)S),$$

where $A + A^T \geq 0$ and S approximates the first derivative at the boundary. In this case, S can be chosen to be accurate of order $p+1$ instead of p and the global accuracy increases from $p+1$ to $p+2$ for pointwise-stable discretizations [4, 31, 50].

Several attempts to include the boundary conditions were made after the construction of the SBP finite difference operator. Injection of the boundary values destroy the SBP properties and stability is restricted to low-order accurate schemes. An orthonormal projection method which preserves the SBP properties was proposed in [41, 42], but is not in practical use because of other complications [28, 30]. The current state-of-the art method for imposing the boundary conditions was proposed by Carpenter et al. in [3] and has become known as the Simultaneous Approximation Term (SAT). Together, the SBP-SAT technique provides a method for constructing stable and high-order accurate approximations of IBVPs.

2.1 Initial boundary value problems

Analyzing the stability requirements for a full time and space discretization is difficult. The analysis can be simplified by only discretizing in space while keeping time continuous. The stability analysis can then be done by using the energy method which is applicable to complicated problems. Such a semi-discretization is called a method of lines [47].

2.1.1 Well-posedness of the continuous problem

The semi-discrete energy estimates are closely related to well-posedness of the continuous problem. One of the earliest definitions of well-posedness were given by Hadamard [16] in the 1920's and can be stated as;

Definition 2.2 (Hadamard)**.** A problem is called well-posed if

1. A solution exists
2. The solution is unique
3. The solution depends smoothly on the data of the problem

The two first statements are obvious for a problem to be computable. The third statement is somewhat vaguely formulated. In Hadamard's original texts, data refers to everything from initial and boundary data to the boundary conditions. Even so, it is clear that such a definition is necessary from a numerical point of view. Every numerical computation produces discretization and round-off errors. These errors can be thought of as data of the problem, and perturbations due to finite precision arithmetic can not be allowed to affect the solution too much.

When studying finite difference discretizations of IBVPs, Kreiss [25] made another definition of well-posedness which became very influential for numerical solutions of PDEs. The definition can be stated as;

Definition 2.3 (Kreiss)**.** A homogeneous IBVP is well-posed if a unique solution u exists and satisfies the energy estimate

$$||u|| \leq K_c e^{\alpha_c t} ||f||, \quad \forall t > 0,$$

where f is the initial data. The parameters K_c and α_c are not allowed to depend on neither t nor f.

By the principle of Duhamel, it is sufficient to study the homogeneous problem since well-posedness of the inhomogeneous problem follows. Moreover, the boundary conditions can also be assumed to be homogeneous [15]. Definition 2.3 quantified the vague definition of Hadamard, and also allowed the solution to be stable against lower-order perturbations. The later property has

extensive use in numerics since non-linear and variable coefficient problems can be treated using linearizations and localizations [22].

2.1.2 Stability of the semi-discrete problem

The definition of Kreiss did not only improve the theory of PDEs in general, it also suggested a method for proving stability of semi-discretizations. The same reasoning can namely be applied in the discrete sense as described in;

Definition 2.4 (Kreiss)**.** A semi-discretization of a homogeneous IBVP is called stable if the discrete solution u_h satisfies the energy estimate

$$||u_h|| \leq K_d e^{\alpha_d t} ||f||, \quad \forall t > 0,$$

where f is the initial data. The parameters K_d and α_d are not allowed to depend on neither t nor f.

Kreiss and Wu [25] showed that when time is kept continuous and a space discretization is stable according to definition 2.4, a Runge-Kutta time integration scheme can be used to integrate the solution in time while maintaining stability.

The outlined procedure of assuming that there is no forcing function and that the boundary conditions are homogeneous gives the most basic sufficient requirements of well-posedness and stability. There are other definitions where the data of the problem is included in the estimates, in which case the continuous problem is called strongly well-posed and the semi-discretization is called strongly stable. Moreover, the semi-discrete problem is called strictly stable if $\alpha_d = \alpha_c + O(\Delta x)$. More details on the definitions and their usage can be found in [15, 36, 39].

We can now exemplify the whole idea of the SBP-SAT method by considering the advection equation with wavespeed $\bar{u} > 0$,

$$\begin{aligned} u_t + \bar{u} u_x &= 0, \qquad 0 \leq x \leq 1, \\ u(x,0) &= f(x), \\ u(0,t) &= g_L(t). \end{aligned} \tag{2.4}$$

Assuming that a unique solution exists, we let $g_L = 0$ and integrate (2.4) over the spatial domain. We obtain

$$\frac{d}{dt}||u||^2 = -\bar{u} u(1,t)^2 \leq 0,$$

which leads to an energy estimate and hence (2.4) is well-posed. An SBP-SAT discretization of (2.4) can be written as

$$\frac{d}{dt} u_h + \bar{u} D_1 u_h = \sigma P^{-1} e_0 (e_0^T u_h - g_L(t)) \tag{2.5}$$

where $e_0 = [1,0,\ldots,0]^T$. The parameter σ has to be determined such that (2.5) is stable in the norm defined by P. By multiplying (2.5) with $u_h^T P$, assuming $g_L = 0$, we get

$$\frac{d}{dt}||u_h||^2 = (\bar{u}+2\sigma)u_h^T E_0 u_h - \bar{u}u_h^T E_N u_h \tag{2.6}$$

and a discrete energy estimate is obtained for $\sigma \leq -\bar{u}/2$. For those values of σ, the scheme is stable. Note that there is no restriction on the order of accuracy for stability in the energy estimate (2.6). Once a discrete energy estimate has been obtained, the same requirements are valid for all orders of accuracy.

The construction of stable boundary procedures for the compressible Navier–Stokes equations with Robin solid wall boundary conditions is the topic of paper III.

2.2 Coupled problems

To study complex flow phenomena, such as conjugate heat transfer, the flow equations need to be coupled with the equations for heat transfer [17, 8, 45]. For model problems, well-posed coupling conditions can be derived using the standard energy method. When the coupling conditions are derived from first principles of physics, the energy method in its standard setting might be insufficient. The reason is that the energy estimates are derived in the L^2-norm which might not capture the physics of the problem. A simple example is the coupled heat equations in one dimension, given by

$$\begin{aligned} u_t &= \alpha_L u_{xx}, & -1 \leq x \leq 0, \\ v_t &= \alpha_R v_{xx}, & 0 \leq x \leq 1, \\ u(-1,t) &= g_L(t), & v(1,t) = g_R(t), \\ u(0,t) &= v(0,t), & \kappa_L u_x(0,t) = \kappa_R v_x(0,t), \end{aligned}$$

where $\alpha_{L,R} = \frac{\kappa_{L,R}}{c_{L,R}\rho_{L,R}}$ are the thermal diffusivities and $\kappa_{L,R}$, $c_{L,R}$, and $\rho_{L,R}$ are the thermal conductivities, specific heat capacities, and densities, respectively. The coupling conditions require continuity of temperature and heat fluxes. In order to obtain an energy estimate, it is necessary to modify the norms as

$$||u||_L^2 = \int_{-1}^{0} u^2 \delta_L dx, \quad ||v||_R^2 = \int_{0}^{1} v^2 \delta_R dx,$$

where $\delta_{L,R} > 0$ are to be determined. The energy method (assuming $g_L = g_R = 0$) results in

$$\frac{d}{dt}(||u||_L^2 + ||v||_R^2) + 2\alpha_L||u_x||_L^2 + 2\alpha_R||v_x||_R^2 = [\delta_L \alpha_L u u_x - \delta_R \alpha_R v v_x]_{x=0}. \tag{2.7}$$

To obtain an energy estimate, using the interface conditions, it is required that $\delta_{L,R} = c_{L,R}\rho_{L,R}$ since then (2.7) reduces to

$$\frac{d}{dt}(||u||_L^2 + ||v||_R^2) + 2\alpha_L||u_x||_L^2 + 2\alpha_R||v_x||_R^2 = [(\kappa_L u_x - \kappa_R v_x)u]_{x=0} = 0,$$

and an energy estimate is obtained.

The modifications of the norms are also seen in the discretization of the coupled problem. A discretization using the SBP-SAT method can be written as

$$\begin{aligned}
\frac{d}{dt}u_h &= \alpha_L D_1^2 u_h + \sigma_1 P^{-1} D_1^T e_0 (e_0^T u_h - g_L) \\
&\quad + \sigma_2 P^{-1} D_1^T e_N (e_N^T u_h - e_0^T v_h) + \sigma_3 P^{-1} e_N (\kappa_L e_N^T (D_1 u_h) - \kappa_R e_0^T (D_1 v_h)) \\
\frac{d}{dt}v_h &= \alpha_R D_1^2 v_h + \tau_1 P^{-1} D_1^T e_N (e_N^T v_h - g_R) \\
&\quad + \tau_2 P^{-1} D_1^T e_0 (e_0^T v_h - e_N^T u_h) + \tau_3 P^{-1} e_0 (\kappa_R e_0^T (D_1 v_h) - \kappa_L e_N^T (D_1 u_h))
\end{aligned} \tag{2.8}$$

and we have to choose $\sigma_{1,2,3}$ and $\tau_{1,2,3}$ such that the scheme is stable. For simplicity, we have assumed that both domains have the same number of grid points since then the same operators can be used in both domains. This is to simplify the notation and in general the domains can have different discretizations. Since a modified norm was required to obtain an energy estimate in the continuous case, the same modification is required to obtain a discrete energy estimate. The modified discrete norms are defined analogously as

$$||u_h||_L^2 = \delta_L u_h^T P u_h, \quad ||v_h||_R^2 = \delta_R v_h^T P v_h,$$

with $\delta_{L,R}$ determined from the continuous energy estimate. To highlight the relation to the continuous energy estimate, we consider only the interface terms and apply the modified energy method with general $\delta_{L,R}$. We get

$$\frac{d}{dt}(||u_h||_L^2 + ||v_h||_R^2) + 2\alpha_L||D_1 u_h||_L^2 + 2\alpha_R||D_1 v_h||_R^2 = q_h^T M q_h,$$

where $q_h = [e_N^T u_h, e_0^T v_h, e_N^T (D_1 u_h), e_0^T (D_1 v_h)]^T$ and

$$M = \begin{bmatrix} 0 & 0 & m_1 & m_2 \\ 0 & 0 & m_3 & m_4 \\ m_1 & m_3 & 0 & 0 \\ m_2 & m_4 & 0 & 0 \end{bmatrix},$$

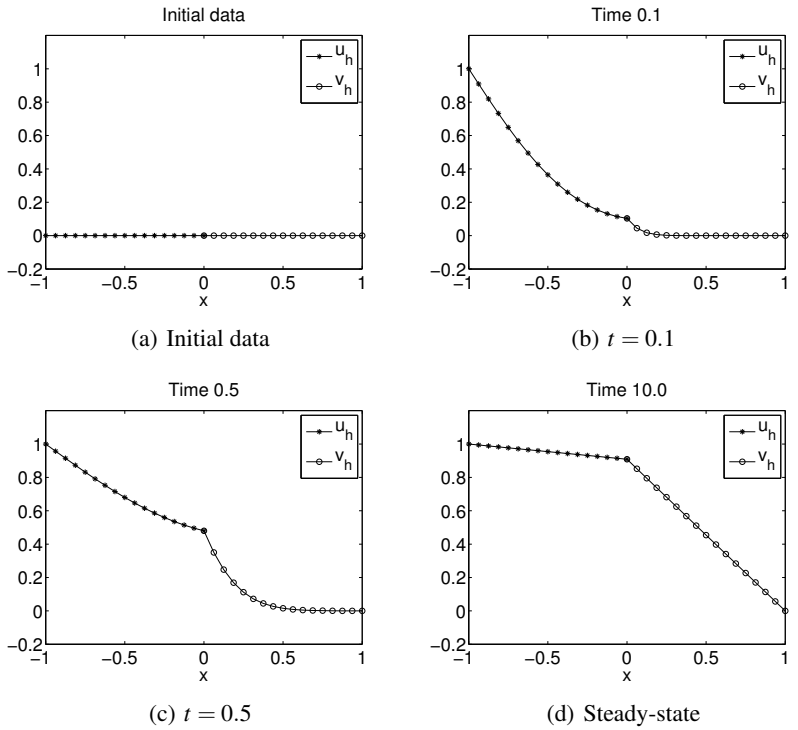
with

$$\begin{aligned}
m_1 &= (\alpha_L + \sigma_2 + \sigma_3 \kappa_L)\delta_L, \quad & m_2 &= -\sigma_3 \delta_L \kappa_R - \tau_2 \delta_R, \\
m_3 &= -\sigma_2 \delta_L - \tau_3 \delta_R \kappa_L, & m_4 &= (-\alpha_R + \tau_2 + \tau_3 \kappa_R)\delta_R.
\end{aligned}$$

In order to obtain an energy estimate, it is required that all parameters are chosen such that $M \leq 0$. Since the main diagonal of M consists of zeros, the only option is to choose the parameters such that $m_{1,2,3,4} = 0$. A little bit of algebra shows that this requirement is possible if, and only if,

$$\frac{\delta_L}{\delta_R} = \frac{c_L \rho_L}{c_R \rho_R},$$

which is satisfied by the choices of $\delta_{L,R}$ from the continuous energy estimate. Thus, if a modified norm is required to obtain an energy estimate in the continuous case, the same modification has to be done to the discrete norm. An example of an implementation of the scheme (2.8) can be seen in Figure 2.2, where we have chosen the problem parameters such that $\alpha_L/\alpha_R = \kappa_L/\kappa_R = 10$.



(a) Initial data (b) $t = 0.1$

(c) $t = 0.5$ (d) Steady-state

Figure 2.2. A sequence of solutions for two coupled heat equations with different problem parameters

In Figure 2.2, the initial data did not match the boundary data at the left boundary. This causes instabilities for schemes with strong implementation of the boundary conditions. With weak boundary conditions and energy stability, the solution attains the boundary value and the scheme remains stable throughout the computation. In this example, we have used 33 grid points in each subdomain and second-order accurate SBP operators.

In paper I and paper IV we investigate coupling procedures for computing conjugate heat transfer problems. In the first case for a one-dimensional model problem, and in the second case for the two-dimensional compressible Navier–Stokes equations. In paper II, the coupling procedure itself is studied using model problems.

3. Functionals and dual problems

The solution of the governing equations might not be the output of primary interest in many CFD applications. Of equal, or even greater, importance is the computation of functionals from the solution. In general, a functional is defined as any map from a vector space V into the underlying scalar field $\mathbb{K}$. Every vector space has an associated vector space called its dual (or adjoint) space. The dual space is denoted by V^* and is defined as the space of all linear functionals $V \to \mathbb{K}$.

The adjoint, or dual, operator L^* of a linear operator L is the (unique) operator satisfying

$$(v, Lu)_V = (L^* v, u)_V, \tag{3.1}$$

where $(.,.)_V$ denotes the inner product on the space V. The study of linear functionals and dual spaces is the topic of functional analysis and additional preliminaries can be found in any functional analysis textbook, for example the classical works [43, 44].

In this section, we consider initial boundary value problems of the form

$$\begin{aligned} u_t + \mathscr{L}(u) &= F, \quad && x \in \Omega, \\ \mathscr{B}(u) &= g_\Gamma, && x \in \Gamma \subseteq \partial\Omega, \\ u &= f, && t = 0. \end{aligned} \tag{3.2}$$

For applications in CFD, a linear functional of interest usually represents the lift or drag on a solid body in a fluid, which is computed in terms of an integral of the solution of (3.2). The functional can be represented in terms of an integral inner product as

$$J(u) = (g, u) = \int_\Omega g^T u d\Omega,$$

where g is a weight function. A main complication in CFD is that no physically relevant solutions have compact support in the computational domain. The dual operator is obtained through integration by parts which will introduce boundary terms that must be removed. The dual PDE has thus to be supplied with dual boundary conditions to close the system.

The associated dual problem has been extensively studied [11, 12] and used in the context of error control and adaptive mesh refinement [1, 2, 6, 14, 10, 7] as well as within optimization and control problems [21, 13]. In error control

and mesh adaptation, the dual problem is derived and treated as a variational problem. In optimization and control problems, the dual problem is derived and treated as a sensitivity problem with respect to design parameters. In the end, the two different formulations yield the same dual problem. A similarity for the different areas of applications is that most of them are based on unstructured methods, such as finite elements or discontinuous Galerkin.

3.1 Quadrature accuracy

Only recently was the study of duality introduced to structured methods, such as the SBP-SAT technique. Recall that the SBP operator was constructed to satisfy

$$(v_h, D_1 u_h)_h = u_h^T (E_N - E_0) v_h - (D_1 v_h, u_h)_h,$$

which mimics an integration property, rather than a differentiation property. While the differentiation properties of the SBP operator has been extensively studied and used [46, 49, 32, 50, 20, 38, 5, 33, 29], the integration properties of the matrix P have been much less explored. The integration properties of P was thoroughly investigated by Hicken and Zingg [19]. It was shown that the requirements on P to obtain an accurate SBP operator include, and extend, the Gregory formulas for quadrature rules using equidistant points. Two main results were proven in [19], which are restated here for convenience. The first theorem establishes the accuracy of P as an integration operator;

Theorem 3.1. *Let P be a full, restricted-full, or diagonal mass matrix from an SBP first-derivative operator $D_1 = P^{-1}Q$, which is a $2p$-order accurate approximation to the first derivative in the interior. Then the mass matrix P constitutes a $2p$-order accurate quadrature for integrands $u \in C^{2p}(\Omega)$.*

The second theorem extends the results to include discrete integrands computed from an SBP differentiation;

Theorem 3.2. *Let $D_1 = P^{-1}Q$ be a an SBP first derivative operator with a diagonal mass matrix P and $2p$-order interior accuracy. Then $(v_h, D_1 u_h)_h$ is a $2p$-order accurate approximation of (v, u_x).*

These theorems proved in summary that it is possible to retain the full order of accuracy when computing integrals from an SBP discretization, even with a diagonal P.

3.2 Dual consistency

For IBVPs, it is not sufficient to integrate the solution obtained by an SBP-SAT discretization using P to obtain a functional of $2p$-order accuracy. It was shown in [18] that an additional property of the discretization was required—the so called dual consistency property. The main result in [18] extends the results in [19] to include SBP-SAT solutions to IBVPs. Even though the solution u_h to an IBVP using SBP-SAT is accurate of order $p+1$ when using a diagonal P, any linear functional of u_h is accurate of order $2p$ when integrated using P, if the discretization is dual consistent.

As suggested by the name, dual consistency requires that the discretization of the primal problem is also a consistent approximation of the dual problem. In order to construct a dual consistent discretization, one first have to derive the dual problem and work with both the primal and dual problems simultaneously. To obtain the dual differential operator we consider the linear, or linearized, Cauchy problem,

$$\begin{aligned} u_t + Lu &= f, & x \in \Omega, \\ u &= 0, & t = 0, \\ J(u) &= (g,u), \end{aligned}$$

where $J(u)$ is a linear functional of interest. We seek a function θ, in some appropriate function space, such that

$$\int_0^T J(u)dt = \int_0^T (\theta, f)dt.$$

Using integration by parts, we can write

$$\begin{aligned} \int_0^T J(u)dt &= \int_0^T J(u)dt - \int_0^T (\theta, u_t + Lu - f)dt \\ &= \int_0^T (\theta_t - L^*\theta + g, u)dt - [(\theta,u)]_{t=T} + \int_0^T (\theta, f)dt \end{aligned}$$

and it is clear that $\theta = 0$ at $t = T$ is needed, and that θ has to satisfy the dual equation $-\theta_t + L^*\theta = g$. The time transform $\tau = T - t$ is usually introduced, and the dual Cauchy problem becomes

$$\begin{aligned} \theta_\tau + L^*\theta &= g, & x \in \Omega, \\ \theta &= 0, & \tau = 0. \end{aligned}$$

The situation is more complicated for IBVPs. Since the primal equation does not have compact support in general, the boundary terms resulting from the

integration by parts procedure has to be properly taken care of by the homogeneous primal boundary conditions. The dual boundary conditions are defined as the minimal set of homogeneous conditions such that the boundary terms vanish after the homogeneous primal boundary conditions have been applied. Still, one needs to investigate the well-posedness of the dual equation with the resulting dual boundary conditions. A well-posed set of boundary conditions for the primal problem does not necessary lead to a well-posed dual problem.

A discretization of a problem with a functional of interest can be written as

$$\begin{aligned} \frac{d}{dt}u_h + L_h u_h &= f, \\ J_h(u_h) &= (g, u_h)_h, \end{aligned} \tag{3.3}$$

where the entire spatial discretization, including the boundary conditions, has been collected into the discrete operator L_h. Recall that the inner product is defined as

$$(v_h, u_h)_h = v_h^T P u_h \tag{3.4}$$

in an SBP-SAT framework. The discrete adjoint operator L_h^* is defined, analogously to (3.1), as the unique operator satisfying

$$(v_h, L_h u_h)_h = (L_h^* v_h, u_h)_h. \tag{3.5}$$

The discrete adjoint operator can hence be explicitly computed, using (3.4) and (3.5), as

$$L_h^* = P^{-1} L_h^T P. \tag{3.6}$$

The discrete dual problem is obtained analogously to the continuous case by finding θ_h such that $\int_0^T J_h(u_h)dt = \int_0^T (\theta_h, f)dt$. Integration by parts and (3.6) gives

$$\begin{aligned} &\int_0^T J_h(u_h)dt = \int_0^T (g, u_h)_h dt - \int_0^T (\theta_h, \frac{d}{dt}u_h + L_h u_h - f)_h dt \\ &= \int_0^T (\frac{d}{dt}\theta_h - L_h^*\theta_h + g, u_h)_h dt - [(\theta_h, u_h)_h]_{t=T} + \int_0^T (\theta_h, f)_h dt \end{aligned}$$

and hence the θ_h has to satisfy the discrete dual problem

$$\begin{aligned} \frac{d}{d\tau}\theta_h + L_h^*\theta_h &= g, \\ \theta_h &= 0, \quad \tau = 0, \end{aligned}$$

where $\tau = T - t$. Dual consistency can now be defined in terms of L_h^* and L^*;

Definition 3.3. A discretization is called dual consistent if L_h^* is a consistent approximation of L^* and the continuous dual boundary conditions.

The above definition is not specific for SBP-SAT discretizations. Any discretization which can be written in the form (3.3) is applicable. The SBP-SAT technique is particularly well-suited for this framework because of the well-defined inner product and operator form.

It is common, in optimization for example, that continuous and discrete adjoint methods are distinguished [34, 35, 9]. This is because the discrete adjoint operator does not approximate the continuous adjoint operator and boundary conditions in general. In the SBP-SAT framework, the dual consistency property can allow for very efficient use of adjoint based techniques due to the unification of the continuous and discrete adjoints. SBP-SAT is not the only method which offers consistency with the dual equations. It was shown that, for example, the discontinuous Galerkin method can also exhibit this property [27, 40].

The dual consistency property can be easily exemplified using the model problem (2.4). Dual consistency does not depend on any data of the problem but only the differential operator and the form of the boundary conditions. We hence consider the inhomogeneous problem with homogeneous boundary and initial conditions,

$$\begin{aligned} u_t + \bar{u}u_x &= f, \qquad 0 \leq x \leq 1 \\ u(0,t) &= 0, \\ u(x,0) &= 0, \\ J(u) &= (g,u), \end{aligned} \tag{3.7}$$

where $J(u)$ is a linear functional of interest. We seek a function θ so that $\int_0^T J(u)dt = \int_0^T (\theta, f)dt$ and integration by parts gives

$$\begin{aligned} \int_0^T J(u)dt &= \int_0^T J(u)dt - \int_0^T (\theta, u_t + \bar{u}u_x - f)dt \\ &= \int_0^T (\theta_t + \bar{u}\theta_x + g, u)dt - \int_0^1 [\theta u]_{t=T}dx - \int_0^T [\bar{u}\theta u]_{x=1}dt + \int_0^T (\theta, f)dt. \end{aligned}$$

It is clear that θ has to satisfy the dual problem

$$\begin{aligned} \theta_\tau - \bar{u}\theta_x &= g, \quad 0 \leq x \leq 1, \\ \theta(1,\tau) &= 0, \\ \theta(x,0) &= 0, \end{aligned} \tag{3.8}$$

where we have introduced the time transform $\tau = T - t$.

The model problem (3.7) can be discretized as

$$\begin{aligned} \frac{d}{dt}u_h + \bar{u}D_1 u_h &= \sigma P^{-1}(e_0^T u_h - 0)e_0 + f, \\ J_h(u_h) &= (g, u_h)_h, \end{aligned} \tag{3.9}$$

and the parameter σ has to be determined so that the scheme is not only stable, but also a consistent approximation of the dual problem (3.8). It is convenient to rewrite (3.9) in operator form as

$$\frac{d}{dt}u_h + L_h u_h = f,$$

where the spatial discretization, including the boundary condition, is included in the operator

$$L_h = \bar{u}D_1 - \sigma P^{-1}E_0.$$

The discrete dual operator can be directly computed as

$$L_h^* = P^{-1}L_h^T P = -\bar{u}D_1 + \bar{u}P^{-1}E_N - (\sigma + \bar{u})P^{-1}E_0, \tag{3.10}$$

and it is seen that L_h^* imposes a boundary condition at $x = 0$, due to the last term in (3.10), unless $\sigma = -\bar{u}$. With $\sigma = -\bar{u}$, the discrete dual problem becomes

$$\frac{d}{d\tau}\theta_h - \bar{u}D_1\theta_h = -\bar{u}P^{-1}E_N\theta_h + g,$$

which is a consistent approximation of the dual problem (3.8). Since $\sigma = -\bar{u}$ does not contradict the stability condition ($\sigma \leq -\bar{u}/2$), the scheme is both stable and dual consistent. In Table 3.1 we show the convergence rates q for the solution and the functionals, together with the functional error, using the dual inconsistent and consistent schemes.

Table 3.1. *Convergence rates q, and functional errors for the dual inconsistent and consistent schemes*

5th-order ($2p = 8$)						
	$\sigma = -1/2$			$\sigma = -1$		
N	$q(u_h)$	$q(J_h(u_h))$	Error	$q(u_h)$	$q(J_h(u_h))$	Error
96	4.58	4.51	1.87e-05	5.14	8.20	7.54e-09
128	4.87	4.80	3.02e-06	5.34	7.96	2.71e-10
160	4.97	4.91	7.58e-07	5.41	8.02	2.74e-11
192	5.02	4.97	2.53e-07	5.44	8.06	4.58e-12
224	5.05	5.01	1.02e-07	5.46	8.21	1.05e-12
256	5.06	5.04	4.72e-08	5.46	8.62	2.97e-13

As we can see from Table 3.1, the convergence rate for the linear functional increases from $p+1$ to $2p$ when using the dual consistent discretization. Also

notice that dual consistency is merely a choice of parameters. The solution of the dual problem is never required and hence the increased rate of convergence for linear functionals comes at no extra computational cost.

In paper V we establish the dual consistency theory for time-dependent problems, and relate the dual consistency property to stability using several model problems of different types. A general proof is presented which shows that stable and dual consistent SBP-SAT schemes produces superconvergent linear integral functionals. In paper VI we extend the theory to include advanced boundary conditions which further enhances the performance of dual consistent schemes.

4. Summary of papers

4.1 Contributions

The ideas of the papers in this thesis have been developed in close collaboration between the authors. The papers have been written by the author of this thesis. The computations in the papers have been performed by the author of this thesis. The analysis in the papers have been done to large extent by the author of this thesis in close collaboration with the co-author.

4.2 Paper I

J. Lindström and J. Nordström. A stable and high-order accurate conjugate heat transfer problem. *Journal of Computational Physics, 229(14):5440–5456, 2010.*

This paper was a first attempt to compute conjugate heat transfer problems using the SBP-SAT framework. In previous work, the coupling procedures have been focused on multi-block couplings to split the computational domain. For conjugate heat transfer problems, not only is the domain split, there are also different governing equations in the blocks describing the fluid and solid, respectively.

A one-dimensional model problem was analyzed. An incompletely parabolic system of equations was coupled to the scalar heat equation and well-posed interface conditions were derived for the continuous problem. The coupled problem was discretized and it was shown how to construct an SAT so that the coupling is stable, and that the target high-order accuracy was obtained.

The stable discrete coupling was derived as a function of one parameter describing the weight between Dirichlet and Neumann conditions, showing that there are no restrictions on how the coupling is done. The results extends earlier results where restrictions on the coupling were required for stability.

The spectral properties of the discretization were investigated as a function of the interface parameter and it was shown that both the rate of convergence to steady-state as well as the stiffness of the coupled system could be enhanced compared to having pure Dirichlet or Neumann conditions.

4.3 Paper II

J. Berg and J. Nordström. Spectral analysis of the continuous and discretized heat and advection equation on single and multiple domains. *Applied Numerical Mathematics, 62(11):1620–1638, 2012.*

To obtain further insights in how numerical coupling procedures affect the overall discretization, two model problems were investigated. Most physical problems consist of advective and/or diffusive terms which have very different mathematical and numerical properties. We hence considered the advection and heat equation on single and multiple domains. This was done to see which effects the multi-block coupling have, compared to a single domain discretization. Second-order accurate SBP operators were used since they allow analytic computations of spectral properties.

For the heat equation, we derived a closed form expression of the eigenvalues for the discrete single domain operator and showed asymptotical second-order convergence of all discrete eigenvalues. For the multi-block domain we showed that the eigenvalues from the single domain operator were included in the set of eigenvalues of the multi-block operator. The stable coupling conditions were derived as a function of one coupling parameter, similarly as in paper I, for which the discretization properties were studied.

For the advection equation, we showed how the eigenvalues of the multi-block operator are again included in the set of eigenvalues of the single domain operator. The multi-block coupling was derived as a function of one semi-bounded parameter for which the discretization is both stable and conservative. Two different values of the parameter could be distinguished. One value which gives minimal interface dissipation, and another which gives a fully upwinded scheme. It was shown by several examples that the upwinded interface treatment is the preferred choice since it improves the errors, stiffness, and rate of convergence to steady-state. In the latter case, adding several interfaces can enhance the convergence rate to steady-state by several orders of magnitude.

4.4 Paper III

J. Berg and J. Nordström. Stable Robin solid wall boundary conditions for the Navier–Stokes equations. *Journal of Computational Physics, 230(19):7519–7532, 2011.*

There are multiple choices of well-posed solid wall boundary conditions for the compressible Navier–Stokes equations. The most commonly used ones are

the no-slip conditions for the velocity with an isothermal or adiabatic temperature condition. These boundary conditions make sure that there are no velocities in neither the normal nor tangential directions, and that the temperature or temperature gradient is specified. It is well-known that the no-slip conditions are accurate as long as the characteristic length scale is large enough. For flows on the micro or nano scale, molecular interactions have to be taken into account, and the Navier–Stokes equations do no longer give an accurate description of the physics. The effects of molecular dynamics can be modeled by slip-flow boundary conditions where the tangential velocities are allowed to be non-zero.

All of the above mentioned boundary conditions can be represented by Robin solid wall boundary conditions on the tangential velocity and temperature. This allows for a transition from no-slip to slip, and from isothermal to adiabatic, by varying parameters. We have proved that the SBP-SAT method can be made stable for all choices of parameters, using sharp energy estimates. All physically relevant solid wall boundary conditions for the compressible Navier–Stokes equations are thus contained within one uniform, energy stable, formulation.

4.5 Paper IV

J. Nordström and J. Berg. Conjugate heat transfer for the unsteady compressible Navier–Stokes equations using a multi-block coupling. *Accepted for publication in Computers & Fluids, 2012.*

There are two possible choices for how to compute conjugate heat transfer problems: 1) the Navier–Stokes equations are coupled to the heat equation, and 2) the Navier–Stokes equations themselves govern heat transfer in the solid. The first is the most obvious choice due to the simplicity of the scalar heat equation. The latter is common for incompressible fluids because the energy component is decoupled from the momentum, and reduces exactly to the heat equation for zero velocities. For compressible fluids, the latter choice is less explored since stability and accuracy become problematic.

We used a modified multi-block coupling, where only the temperature is coupled over the interface, and let the compressible Navier–Stokes equations govern heat transfer also in the solid region. In the continuous case, we showed how to scale and choose the coefficients in the energy component of the Navier–Stokes equations, so that it becomes as similar to the heat equation as possible. Well-posedness of the modified multi-block coupling was shown using energy estimates in a modified norm.

In the discrete case, we showed that the coupling can be made stable using the same modified norm. Computations using both approaches were performed and it was shown that the differences can be made very small.

4.6 Paper V

J. Berg and J. Nordström. Superconvergent functional output for time-dependent problems using finite differences on summation-by-parts form. *Journal of Computational Physics, 231(20):6846–6860, 2012.*

The theory of dual consistency and functional superconvergence for SBP-SAT discretizations was first derived for steady problems. In this paper, we extended the theory to time-dependent problems and related dual consistency to stability. We gave a general proof that dual consistency and stability implies superconvergence for linear (integral) functionals. Several model problems of different kinds were analyzed. It was shown how to construct schemes which are stable and dual consistent, and that superconvergence was obtained for all cases.

4.7 Paper VI

J. Berg and J. Nordström. On the impact of boundary conditions on dual consistent finite difference discretizations. *Accepted for publication in Journal of Computational Physics, 2012.*

In paper V, the model PDEs were supplied with Dirichlet boundary conditions to simplify the analysis in the continuous case. Dirichlet boundary conditions automatically ensures that both the primal and dual problems are well-posed. The discretization, however, became more complicated as it was required to reduce the equations to first-order form to derive stability conditions. In realistic applications, Dirichlet boundary conditions are rarely suitable at far-field boundaries. It is well-known that they give large reflections which eventually will pollute the whole solution unless exact boundary data is known. Other kind of boundary conditions can significantly enhance both the stability and accuracy of a numerical scheme.

We considered a linear incompletely parabolic system of PDEs in one dimension. The boundary conditions of far-field type were derived using energy

estimates, under the restriction that both the primal and dual problems were well-posed. By simultaneously considering the primal and dual problems, the amount of free parameters could be reduced, which allowed the construction of new advanced boundary conditions.

The equations were discretized using the SBP-SAT technique, and it was shown that the construction of the continuous boundary conditions are sufficient for both stability and dual consistency. In fact, with the new boundary conditions, stability and dual consistency are equivalent. Several computations were performed with the new boundary conditions, and it was shown that they provide both error boundedness in time, fast convergence to steady-state, and superconvergence of linear integral functionals.

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6. Summary in Swedish

Stabila finita differensmetoder med hög noggrannhetsordning för multifysik- och flödesproblem

Många problem inom teknik och naturvetenskap, och även inom andra områden, kan modelleras med hjälp av partiella differentialekvationer (PDE:er). Några exempel är dynamiken hos fluider och elektromagnetisk vågutbredning, men även problem från aktiemarknaden och trafikstockningar kan beskrivas med PDE:er. I allmänhet finns inga generella metoder för att hitta exakta lösningar till dessa problem. Även i de fall där det finns exakta lösningar så är de i allmänhet för komplexa för att vara praktiskt användbara. Numeriska metoder är därför ofta nödvändiga.

Under de senaste årtiondena har datorerna utvecklats till den grad att numeriska simuleringar har etablerat sig som ett av vetenskapens fundament, likvärdigt med teori och experiment. Den ökade användningen av datorer är inte enbart tack vare att hårdvaran har blivit snabbare och effektivare. Algoritmerna som används för beräkningar har även de utvecklats i samma takt. Den ökade användningen av datorsimuleringar ställer höga krav på algoritmerna. Bra hårdvara är betydelselös om algoritmen som används är ineffektiv eller inte beräknar ett korrekt resultat.

Det finns en uppsjö av olika metoder för att lösa PDE:er. Några av de vanligaste är finita volymsmetoden, finita elementmetoden, och den som är huvudfokus i den här avhandlingen – finita differensmetoden. Vilken metod som än används så krävs det att metoden är;

1. Konsistent
2. Stabil
3. Effektiv

I allmänhet är två av de tre ovanstående kraven relativt lätta att åstadkomma. Att metoden är konsistent betyder att den faktiskt löser den PDE vi är intresserade av. Stabilitet betyder att störningar, t.ex. i data eller från diskretiserings- eller avrundningsfel, inte påverkar lösningen alltför mycket. Effektivitet betyder att metoden levererar en lösning inom rimlig tid. De flesta metoder som används är i praktiken är konsistenta. Däremot är långt ifrån alla metoder som används stabila och effektiva. En konsistent och stabil numerisk metod har ofta en låg noggrannhetsordning och är därmed ineffektiv, eftersom det krävs hög upplösning för ett noggrant resultat. En konsistent metod med hög noggrannhetsordning är ofta instabil.

Finita differensmetoder är i sitt grundutförande konsistenta och effektiva. Effektiviteten kommer av att det är lätt att åstadkomma hög noggrannhetsordning, samt att de lämpar sig väl för implementering på datorer. Ett stort problem är stabilitet. För att komma till rätta med stabilitetsproblemen har finita differensmetoder på partiell summationsform (eng. summation-by-parts, SBP) utvecklats. En SBP-operator är i grunden en central differensoperator som har modifierats för att vara ensidig vid ränderna. SBP-egenskapen i sig är tillräcklig för att varje linjärt välställt Cauchy-problem ska ha en stabil diskretisering.

För initial- och randvillkorsproblem (eng. initial boundary value problems, IBVP) är situationen lite mer komplicerad. De flesta PDE:er av fysikaliskt intresse, t.ex. Navier-Stokes ekvationer, kräver randvillkor för att vara väldefinierade. SBP-metodiken i sig har ingen hantering av randvillkor utan dessa måste läggas till separat. Den mest användbara metoden är att lägga till randvillkoren svagt, genom en så kallad SAT (eng. simultaneous approximation term). Tillsammans ger SBP-SAT ett ramverk för att konstruera konsistenta och stabila finita differensapproximationer av linjärt välställda IBVP, där noggrannhetsordningen inte är begränsad av stabilitetskrav.

Den här avhandlingen fokuserar på stabila och högre ordningens SBP-SAT-approximationer av olika IBVP som förekommer inom beräkningsfluiddynamik. I åtanke finns speciellt Navier-Stokes ekvationer samt multifysikproblem inklusive konjugerad värmeöverföring. Avhandlingen kan delas in i två delar. Den första delen består av artikel I–IV. I dessa utvecklas SBP-SAT-tekniken för kopplade problem samt randvillkorshantering för Navier–Stokes ekvationer. Det visas hur SBP-SAT används för att koppla ihop olika fysikmodeller och vilka egenskaper hos diskretiseringen som ändras vid kopplingen. Väggrandvillkor för Navier-Stokes ekvationer som leder till välställdhet för det kontinuerliga problemet härleds, tillsammans med stabilitet för det diskreta. Väggrandvillkoren är formulerade så att alla relevanta fysikaliska randvillkor, t.ex. no-slip, slip, isoterma och adiabatiska, finns representerade i en enhetlig formulering som är energistabil med skarpa energiuppskattningar.

I den andra delen, bestående av artikel V–VI, utvecklas SBP-SAT-tekniken för hantering av duala problem. Dualkonsistens relateras till stabilitet vilket resulterar i superkonvergenta linjära integralfunktionaler. Genom att samtidigt betrakta välställdhet hos det primära och duala problemet kan nya avancerade randvillkor härledas, vilka i en SBP-SAT-diskretisering direkt ger stabilitet och dualkonsistens, och därmed superkonvergenta funktionaler.

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