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Stable Numerical Methods with Boundary and Interface Treatment for Applications in Aerodynamics

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Abstract

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In numerical simulations, problems stemming from aerodynamics pose many challenges for the method used. Some of these are addressed in this thesis, such as the fluid interacting with objects, the presence of shocks, and various types of boundary conditions.

Scenarios of the kind mentioned above are described mathematically by initial boundary value problems (IBVPs). We discretize the IBVPs using high order accurate finite difference schemes on summation by parts form (SBP), combined with weakly imposed boundary conditions, a technique called simultaneous approximation term (SAT). By using the energy method, stability can be shown.

The weak implementation is compared to the more commonly used strong implementation, and it is shown that the weak technique enhances the rate of convergence to steady state for problems with solid wall boundary conditions. The analysis is carried out for a linear problem and supported numerically by simulations of the fully non-linear Navier–Stokes equations.

Another aspect of the boundary treatment is observed for fluid structure interaction problems. When exposed to eigenfrequencies, the coupled system starts oscillating, a phenomenon called flutter. We show that the strong implementation sometimes cause instabilities that can be mistaken for flutter.

Most numerical schemes dealing with flows including shocks are first order accurate to avoid spurious oscillations in the solution. By modifying the SBP-SAT technique, a conservative and energy stable scheme is derived where the order of accuracy can be lowered locally. The new scheme is coupled to a shock-capturing scheme and it retains the high accuracy in smooth regions.

For problems with complicated geometry, one strategy is to couple the finite difference method to the finite volume method. We analyze the accuracy of the latter on unstructured grids. For grids of bad quality the truncation error can be of zeroth order, indicating that the method is inconsistent, but we show that some of the accuracy is recovered.

We also consider artificial boundary closures on unbounded domains. Non-reflecting boundary conditions for an incompletely parabolic problem are derived, and it is shown that they yield well-posedness. The SBP-SAT methodology is employed, and we prove that the discretized problem is stable.

Keywords: summation by parts, simultaneous approximation term, accuracy, stability, finite difference methods

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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 S. Eriksson and J. Nordström, Analysis of the order of accuracy for node-centered finite volume schemes, *Applied Numerical Mathematics*, 59(10):2659–2676, 2009.

II J. Nordström and S. Eriksson, Fluid structure interaction problems: the necessity of a well posed, stable and accurate formulation, *Communications in Computational Physics*, 8(5):1111–1138, 2010.

III S. Eriksson, Q. Abbas, and J. Nordström, A stable and conservative method for locally adapting the design order of finite difference schemes, *Journal of Computational Physics*, 230(11):4216–4231, 2011.

IV J. Nordström, S. Eriksson, and P. Eliasson, Weak and strong wall boundary procedures and convergence to steady-state of the Navier–Stokes equations, *Journal of Computational Physics*, 231(14):4867–4884, 2012.

V S. Eriksson and J. Nordström, Exact non-reflecting boundary conditions revisited: well-posedness and stability, Technical report 2012-032, Department of Information Technology, Uppsala University, 2012.

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Contents

1. Introduction

In this thesis the numerical solutions to time-dependent partial differential equations (PDEs) are considered, with the main focus being the implementation of boundary and coupling conditions.

PDEs model numerous natural phenomena, with applications in fields like biology, physics, and engineering. Examples of PDEs include the Navier–Stokes equations which describe the motion of fluids, Maxwell's equations used for classical electromagnetics, and the Schrödinger equation which models quantum dynamic processes.

By providing a time-dependent PDE with an initial condition and boundary conditions it becomes an initial boundary value problem (IBVP). In most cases these equations are too complicated to be solved analytically, and the solution must be approximated using numerical methods. There are numerous different methods for solving PDEs numerically. The most common ones are the finite difference method, the finite element method, and the finite volume method. All of these numerical methods have their own advantages and drawbacks: The finite difference method is straightforward to understand and apply (if one disregards the complicated boundary treatment, which is the topic of this thesis). The finite element method is developed in a more intricate mathematical framework and is together with the finite volume method well suited to handle complicated geometries.

Often it is the boundary conditions in the IBVPs rather than the PDE itself that introduce difficulties, such as cumbersome implementation and instabilities. In this thesis we will use finite difference methods on summation by parts form with weak boundary treatment for solving the IBVPs. This method, hereafter referred to as the SBP-SAT methodology, provides a systematic way of imposing the boundary conditions, yielding an accurate, efficient, and stable numerical scheme.

1.1 Previous work

When a central finite difference stencil is used to approximate the derivatives in an IBVP, the stencil must be modified at the boundaries so that the numerical solution satisfies the boundary conditions. However, even in the absence of boundary conditions, the stencil must be modified since there are no solution values outside the numerical domain. This modification of the scheme, the numerical boundary condition, can be dealt with by extrapolation, or by using one-sided stencils at the boundaries [7, 8]. The summation by parts (SBP) operators are a special form of the latter. The SBP operators were first developed by Kreiss and Scherer [13] for first derivatives, and improved by Strand [28]. Later operators for second derivatives were derived in [4] by Carpenter et al. and developed further in [17] by Mattsson and Nordström.

When imposing the boundary conditions of the IBVP the scheme must be additionally modified. If this is not done with care the stability properties given by the SBP

form can be destroyed. In [2], Carpenter et. al. studied the stability properties of various high order finite difference schemes, with the conclusion that many schemes were not time-stable. As a solution to this problem they introduced a boundary procedure called simultaneous approximation term (SAT) [3], which was an extension of the work by Funaro and Gottlieb in [6]. With the combined use of SBP operators and the SAT boundary procedure, time-stability could be obtained. Other types of boundary procedures that lead to stability exist, see for example [25, 26].

1.2 Well-posedness and stability

An essential key to success when constructing numerical methods, is the study of the continuous problem. If the IBVP is not well-posed, there is no point in trying to find a stable numerical procedure. The concept of well-posedness was introduced by Hadamard [11], and states that a problem is well-posed if

1. a solution exists,
2. the solution is unique, and
3. the solution depends continuously on data.

To show existence can be difficult, (it is actually one of the Millennium Prize Problems, posed by Clay Mathematics Institute in 2000, to prove that a smooth solution exists for the three-dimensional Navier–Stokes equations). In this thesis we assume that a unique solution exists and focus on the third requirement, which is equivalent to limiting the growth of the solution over time, see [9]. (In fact, the second requirement follows from the third one.) The main tools for determining the solution growth are the energy method and the Laplace transform method.

Correspondingly for a numerical method, it is essential that it is consistent (accurate), convergent, and stable. According to the Lax–Richtmyer equivalence theorem, a consistent method (for a linear problem) is convergent if and only if it is stable. Consistency is rather easily accomplished, however to show stability is in many cases non-trivial. We will use the SBP operators and choose eligible SAT terms such that the continuous energy estimates can be mimicked numerically, and stability can be obtained.

2. Stable high order finite difference methods

To explain the numerical procedure and concepts of SBP-SAT, we let the advection equation

$$\begin{aligned} &u_t + u_x = 0, \qquad 0 \le x \le 1, \qquad t \ge 0, \\ &u(x,0) = f(x), \\ &u(0,t) = g(t), \end{aligned} \tag{2.1}$$

serve as our model IBVP. In (2.1), f is the initial value function, g is the boundary data and $u(x,t)$ is the solution. The spatial domain $x \in [0,1]$ is discretized using $N+1$ equidistant grid points, as $x_i = i/N$, where $i = 0,1,\ldots,N$. On this grid the solution $u(x,t)$ is approximated by the time-dependent vector $\mathbf{v} = [\mathbf{v}_0, \mathbf{v}_1, \ldots, \mathbf{v}_N]^T$. By using the SBP-SAT technique, the semi-discrete scheme modeling the IBVP (2.1) is written

$$\begin{aligned} &\mathbf{v}_t + D\mathbf{v} = P^{-1} e_0 \tau (\mathbf{v}_0 - g), \qquad t \ge 0, \\ &\mathbf{v}(0) = \mathbf{f}. \end{aligned} \tag{2.2}$$

The function $f(x)$ is represented by $\mathbf{f} = [\mathbf{f}_0, \mathbf{f}_1, \ldots, \mathbf{f}_N]^T$, such that $\mathbf{f}_i = f(x_i)$. Further, the differentiation operator $\partial/\partial x$ is approximated by the matrix D, and the boundary condition $u - g = 0$ is imposed by the term $P^{-1} e_0 \tau (\mathbf{v}_0 - g)$. The form of D, P, e_0 and τ will described in the following sections.

The procedure of only discretizing the spatial variable is often referred to as the method of lines, see [9, 27], and results in a system of ordinary differential equations. There are many numerical methods for solving ordinary differential equations, and in this thesis we have often used the classical Runge-Kutta method for time discretization.

2.1 Summation by parts operators

The matrix D in (2.2) is a finite difference operator. Such operators are constructed using Taylor expansions so that $(D\mathbf{f})_i \approx f_x'(x_i)$, and can be designed to be more or less accurate. The operator D is on SBP form if it can be written

$$D = P^{-1} Q, \qquad Q + Q^T = E_N - E_0, \qquad P = P^T > 0, \tag{2.3}$$

where $E_0 = \mathrm{diag}(1,0,\ldots,0)$ and $E_N = \mathrm{diag}(0,\ldots,0,1)$. Now consider two arbitrary, smooth functions $a(x), b(x)$, represented discretely by the vectors $\mathbf{a}$, $\mathbf{b}$. The idea behind the summation by parts operators is that they, besides the accuracy demand, should mimic the integration by parts property

$$\int_0^1 a(x) b_x'(x)\, dx = a(1)b(1) - a(0)b(0) - \int_0^1 a_x'(x) b(x)\, dx. \tag{2.4}$$

If D satifies the requirements in (2.3), it will fulfill the summation by parts formula

$$\mathbf{a}^T P(D\mathbf{b}) = \mathbf{a}_N \mathbf{b}_N - \mathbf{a}_0 \mathbf{b}_0 - (D\mathbf{a})^T P\mathbf{b},$$

which is the discrete analogy to (2.4). In the simplest example $D = P^{-1}Q$ is a second order accurate approximation of $\partial/\partial x$ with

$$P = \Delta x \begin{bmatrix} 1/2 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & & 1/2 \end{bmatrix}, \quad Q = \frac{1}{2} \begin{bmatrix} -1 & 1 & & & & \\ -1 & 0 & 1 & & & \\ & \ddots & \ddots & \ddots & & \\ & & -1 & 0 & 1 & \\ & & & -1 & 1 \end{bmatrix}, \quad (2.5)$$

where $\Delta x = 1/N$ is the grid size. Using the P and Q in (2.5) we get

$$(D\mathbf{f})_i = \frac{\mathbf{f}_{i+1} - \mathbf{f}_{i-1}}{2\Delta x} = f_x(x_i) + O(\Delta x^2),$$

$$(D\mathbf{f})_0 = \frac{\mathbf{f}_1 - \mathbf{f}_0}{\Delta x} = f_x(0) + O(\Delta x), \qquad (D\mathbf{f})_N = \frac{\mathbf{f}_N - \mathbf{f}_{N-1}}{\Delta x} = f_x(1) + O(\Delta x),$$

That is, the operator is central in the interior and one-sided at the boundaries. For a diagonal P the resulting difference operator D, with order $2p$ in the interior, must have half the order of accuracy, p, at the boundaries. If the solution obtained using such a D is point-wise bounded, it will be $(p+q)$th order accurate, where $\partial^q/\partial x^q$ is the highest derivative of the PDE, see [7, 8, 31]. The SBP operators are derived for up to eight order of interior accuracy [28], for second derivatives with constant coefficients, see [17], and with variable coefficients, see [12, 16].

2.2 Weak boundary conditions

The SBP operators approximate the derivatives in the PDE. However, the true difficulties arise first when boundary conditions are introduced. The most intuitive way of imposing the boundary conditions is to simply replace the solution value by data at the boundary, with the so called injection method. Consider solving (2.1) numerically using the scheme

$$\begin{aligned} \mathbf{v}_t + D\mathbf{v} &= 0, \qquad t \geq 0, \\ \mathbf{v}(0) &= \mathbf{f}. \end{aligned}$$

Using the injection technique, the above scheme is discretized in time, and after each time step the solution value $\mathbf{v}_0$ is overwritten by $g(t)$. This approach is also referred to as a strong imposition of the boundary conditions, and is widely used. However, for more complicated problems and with higher order accurate difference approximations, stability can not be guaranteed. See for example [3, 15] on how the strong implementation can ruin the stability properties of the scheme.

By relaxing the demand for absolute accuracy at the boundary, stability can be obtained. Consider the scheme in (2.2), where the right-hand side is a penalty term

called the SAT term. The properties of D and P are specified in (2.3), $e_0 = [1,0,\ldots,0]^T$ and τ is a scalar (denoted the penalty parameter). Written out explicitly row by row, the equation is $(\mathbf{v}_i)_t + (D\mathbf{v})_i = 0$, but for the first row we have (for the 2nd order accurate scheme presented in (2.5))

$$(\mathbf{v}_0)_t + \frac{\mathbf{v}_1 - \mathbf{v}_0}{\Delta x} = \frac{2\tau}{\Delta x}(\mathbf{v}_0 - g).$$

Instead of demanding that $\mathbf{v}_0 \equiv g$, the solution is penalized if $\mathbf{v}_0$ is too far from the prescribed data. The SAT term can be viewed as a spring that pulls the solution towards the boundary data, where the quantity $\tau/\Delta x$ determines the strength of the spring.

Since the boundary condition is not fulfilled exactly, this method is referred to as a weak imposition of the boundary conditions. This should however not be viewed as a drawback. On the contrary, the magnitude of the difference $\mathbf{v}_0 - g$ can serve as an indication of how large the discretization error is in the interior. Often the strong boundary procedure results in a less accurate interior solution, as shown in [1].

2.3 Energy estimates

The most prominent property of the SBP-SAT methodology is that energy estimates can be obtained in a systematic way. The basis for this is the mimetic features of the SBP operators and the flexibility of the SAT terms. First we derive an energy estimate for the continuous problem, then the procedure is repeated for the discrete formulation.

2.3.1 The continuous formulation

Consider the IBVP (2.1). To obtain an energy estimate, the PDE is multiplied by u and integrated with respect to x. Integrating by parts yields

$$\frac{d}{dt}\|u\|^2 = u(0,t)^2 - u(1,t)^2, \tag{2.6}$$

where the norm is defined as $\|u\|^2 = \int_0^1 u^2 dx$. To bound the right-hand side of (2.6) the boundary condition in (2.1) is used, and we obtain

$$\frac{d}{dt}\|u\|^2 = g(t)^2 - u(1,t)^2. \tag{2.7}$$

The bounded energy rate (2.7) leads to an energy estimate by time-integration.

2.3.2 The discrete formulation

Consider the semi-discrete scheme (2.2). Recall that $D = P^{-1}Q$, where P and Q possess the properties in (2.3). Multiplying the system of ordinary differential equations in (2.2) by $\mathbf{v}^T P$ from the left (which corresponds to multiplying the continuous equation by u and integrating), and thereafter adding the transpose of the equation to itself,

yields

$$\frac{d}{dt}\|\mathbf{v}\|_P^2 = \mathbf{v}_0^2 - \mathbf{v}_N^2 + 2\tau\mathbf{v}_0(\mathbf{v}_0 - g), \tag{2.8}$$

where the norm is defined as $\|\mathbf{v}\|_P^2 = \mathbf{v}^T P\mathbf{v}$. Having $\tau = 0$ corresponds to not imposing any boundary condition, cf. the continuous case in (2.6). Completing the squares in (2.8) gives

$$\frac{d}{dt}\|\mathbf{v}\|_P^2 = (1+2\tau)\left(\mathbf{v}_0 - \frac{\tau g}{1+2\tau}\right)^2 - \frac{\tau^2 g^2}{1+2\tau} - \mathbf{v}_N^2.$$

The scheme (2.2) is hence stable for $\tau \leq -1/2$. For the special choice $\tau = -1$ the energy rate becomes

$$\frac{d}{dt}\|\mathbf{v}\|_P^2 = g^2 - \mathbf{v}_N^2 - (\mathbf{v}_0 - g)^2. \tag{2.9}$$

Note that (2.9) is an exact numerical representation of (2.7), except for an additional damping term. The damping term is a function of the deviation from the boundary data, and goes to zero as the mesh is refined.

The weak technique for boundary conditions is used in Paper I for the finite volume method, and in Papers II-V for the finite difference method.

2.4 Weak interface coupling

If the computational domain can be transformed smoothly to a square (or cube), the SBP operators can be used in combination with curvilinear grids. This can be achieved without destroying the stability properties (if P is diagonal), see [30].

If the geometry is complex, several domains can be coupled together using SAT interfaces, which is studied in [4, 20, 21]. As an extension of that, the SBP finite difference schemes have also, in [22, 23, 24], been coupled to the finite volume method. Another application is the coupling of regions with different physical properties, as in [14, 19] where the interaction between a fluid and a heat conducting wall is studied.

To exemplify the SAT technique for interfaces, we use the problem (2.1) again. The problem is now discretized with $2(N+1)$ grid points and a SAT interface at $x = 0.5$, such that the numerical scheme becomes

$$\mathbf{v}_t^L + D_L\mathbf{v}^L = P_L^{-1}e_N\tau_L(\mathbf{v}_N^L - \mathbf{v}_0^R), \qquad \mathbf{v}_t^R + D_R\mathbf{v}^R = P_R^{-1}e_0\tau_R(\mathbf{v}_0^R - \mathbf{v}_N^L), \tag{2.10}$$

where we omit the outer boundary condition. The solution in the left part of the domain, $x \in [0,\ 0.5]$, is approximated by v^L and the solution in the right part of the domain, $x \in [0.5,\ 1]$, is approximated by v^R. Correspondingly to e_0, we define $e_N = [0,\ldots,0,1]^T$. The penalty terms in (2.10) force the left solution $\mathbf{v}_N^L$ to the right solution $\mathbf{v}_0^R$, and vice versa, instead of towards a known function g as in (2.2). Note that $\mathbf{v}_N^L$ and $\mathbf{v}_0^R$ are both approximations of the same continuous solution value, $u(0.5,t)$, but that they are not necessarily identical. The SBP operators D_L and D_R in (2.10) can have different orders of accuracy.

To choose the penalty parameters τ_L and τ_R so that the coupled schemes in (2.10) become stable, we derive an energy estimate. The same exercise as for the single-domain scheme is repeated, i.e. the schemes are multiplied from the left by $\mathbf{v}_L^T P_L$ and $\mathbf{v}_R^T P_R$, respectively, we add the transposes, and use the SBP properties (2.3). This leads, after adding the two estimates, to

$$\frac{d}{dt}\left(\|\mathbf{v}^L\|_{P_L}^2+\|\mathbf{v}^R\|_{P_R}^2\right)=(\mathbf{v}_0^L)^2-(\mathbf{v}_N^R)^2+\begin{bmatrix}\mathbf{v}_N^L\\ \mathbf{v}_0^R\end{bmatrix}^T\underbrace{\begin{bmatrix}2\tau_L-1 & -\tau_L-\tau_R\\ -\tau_L-\tau_R & 2\tau_R+1\end{bmatrix}}_{M}\begin{bmatrix}\mathbf{v}_N^L\\ \mathbf{v}_0^R\end{bmatrix}$$

which corresponds to the continuous estimate (2.6). To avoid an energy contribution from the coupling term, the matrix M must be negative semi-definite. This can only be achieved if $\tau_L-\tau_R-1=0$. That requirement is fulfilled if $2\tau_L-1=2\tau_R+1=-\theta$, where $\theta\geq 0$ is a half-bounded parameter, and we obtain

$$\frac{d}{dt}\left(\|\mathbf{v}^L\|_{P_L}^2+\|\mathbf{v}^R\|_{P_R}^2\right)=(\mathbf{v}_0^L)^2-(\mathbf{v}_N^R)^2-\theta\left(\mathbf{v}_N^L-\mathbf{v}_0^R\right)^2.$$

The weak technique for interfaces is used in Paper II and III. In Paper III it is used as a starting point for deriving a new operator, where the double values $\mathbf{v}_N^L$ and $\mathbf{v}_0^R$ are merged into one value. In Paper II it is used for coupling the linearized Euler equation to the spring equation in order to study fluid structure interaction.

3. The Laplace transform method

In the previous section we used the energy method to prove well-posedness. Another, more general, method for examining the well-posedness of a problem is the so called Laplace transform method. This technique can be fruitful not only for showing well-posedness, but also for studying different aspects of the solution behavior. The procedure is described in detail in [5, 9, 18]. Here, as an example, we consider the linear system of PDEs

$$\begin{aligned} U_t + AU_x - BU_{xx} &= 0, \qquad x_L \le x \le x_R, \quad t \ge 0, \\ U(x,0) &= f(x), \\ L_L U(x_L,t) &= g_L(t), \\ L_R U(x_R,t) &= g_R(t), \end{aligned} \tag{3.1}$$

where $f(x)$ is the initial data and $L_{L,R}U(x_{L,R},t) = g_{L,R}$ are the boundary conditions. A and B are matrices, and U is the solution vector. By applying the Laplace transform to (3.1), we obtain a system of ordinary differential equations,

$$\begin{aligned} s\hat{U} + A\hat{U}_x - B\hat{U}_{xx} &= f, \qquad x_L \le x \le x_R, \\ \hat{L}_L\hat{U}(x_L,s) &= \hat{g}_L(s), \\ \hat{L}_R\hat{U}(x_R,s) &= \hat{g}_R(s), \end{aligned} \tag{3.2}$$

where $s = \eta + \xi i$ is the dual variable to time, and where $\hat{U}$ is defined as

$$\hat{U}(x,s) = \mathscr{L}\{U(x,t)\} = \int_0^\infty e^{-st}U(x,t)\,dt, \qquad \mathscr{L}\{U_t'(x,t)\} = s\hat{U}(x,s) - U(x,0).$$

The solution to (3.2) consists of a homogenous part and a particular part, as $\hat{U} = \hat{U}_h + \hat{U}_p$. The particular solution $\hat{U}_p$ (which depends on the data f) is assumed known. For the homogenous part, the ansatz $\hat{U}_h = e^{\kappa x}\psi$ leads to an eigenvalue problem for $\kappa(s)$ and $\psi(s)$ on the form

$$(sI + \kappa A - \kappa^2 B)\psi = 0. \tag{3.3}$$

The eigenvalue problem (3.3) can only have non-trivial solutions $\psi \neq 0$ if the determinant $|sI + \kappa A - \kappa^2 B|$ is zero. Solving the polynomial $|sI + \kappa A - \kappa^2 B| = 0$ for the eigenvalues κ_j, and assuming that the roots κ_j are distinct, gives the general homogeneous solution

$$\hat{U}_h = \sum_j \sigma_j e^{\kappa_j x}\psi_j. \tag{3.4}$$

The coefficients σ_j can be determined using the boundary conditions. The signs of the real parts of the eigenvalues κ_j determine the correct number of boundary conditions

at each boundary. It is shown in [29] that for each negative $\mathrm{Re}(\kappa_j)$ we need one condition at the left boundary, and for each positive $\mathrm{Re}(\kappa_j)$ we need one condition at the right boundary. Consider the homogeneous solution (3.4). By defining

$$\Psi = [\psi_1, \psi_2, \ldots], \qquad K(x) = \mathrm{diag}(e^{\kappa_1 x},\ e^{\kappa_2 x},\ \ldots), \qquad \sigma = [\sigma_1, \sigma_2, \ldots]^T,$$

we can write $\hat{U}_h = \Psi K \sigma$. Further, for the homogenous part of the solution the boundary conditions in (3.2) become $\hat{L}_{L,R}\hat{U}_h = g'_{L,R}$, where $g'_{L,R} = \hat{g}_{L,R} - \hat{L}_{L,R}\hat{U}_p$. Applying these conditions to $\hat{U}_h = \Psi K \sigma$ yields

$$E(s)\sigma = g', \qquad E(s) = \begin{bmatrix} \hat{L}_L \Psi K(x_L) \\ \hat{L}_R \Psi K(x_R) \end{bmatrix},$$

where $g' = [(g'_L)^T, (g'_R)^T]^T$. Each row of the system above corresponds to one boundary condition, and for general boundary conditions the matrix $E(s)$ is full. If $E(s)$ is non-singular we can solve for σ and obtain a unique solution $\hat{U} = \hat{U}_p + \Psi K E(s)^{-1} g'$. We can formally transform back to the time domain, using

$$U(x,t) = \mathscr{L}^{-1}\{\hat{U}(x,s)\} = e^{\eta_0 t}\left(\frac{1}{2\pi}\int_{-\infty}^{+\infty} \hat{U}(x, \eta_0 + i\xi) e^{i\xi t} d\xi\right),$$

where $E(s)$ must be non-singular for $\eta > \eta_0$. The solution does not grow in time if $\eta_0 \leq 0$, and for convergence to steady-state $\eta_0 < 0$ is necessary. The problem is well-posed even if $0 < \eta_0 < \infty$, but then the bound allows for exponential growth and is only permissible for problems involving lower order terms.

The above described technique can also be used for the fully discretized problem, and is then sometimes referred to as GKS-analysis, after a paper by Gustafsson, Kreiss, and Sundström [10], or normal mode analysis, see [9]. We will denote well-posedness obtained in this way; *well-posed in the GKS sense*.

The Laplace technique is used in paper II, IV and V. In paper II it is used to identify the eigenfrequencies of a coupled fluid structure system, and use them as a reference for the numerical solution. In paper IV the decay rate η_0 is computed, which decides the rate at which the solution converges to steady-state. In paper V it is used for showing well-posedness of a problem with non-reflecting boundary conditions.

4. Summary of papers

The content of the papers in the thesis will briefly be reviewed in this section.

4.1 Paper I

S. Eriksson and J. Nordström, Analysis of the order of accuracy for node-centered finite volume schemes, Applied Numerical Mathematics, 59(10):2659–2676, 2009.

The motivation for this work was contradictory observations of the accuracy of the node-centered finite volume method on unstructured grids. We study the problems

$$u_x = F_1, \qquad -u_{xx} = F_2, \tag{4.1}$$

augmented with Dirichlet boundary conditions. The problems are approximated numerically by a finite volume scheme on SBP form, such that

$$P^{-1}\widetilde{Q}\mathbf{v} = \widetilde{\mathbf{F}}_1, \qquad -P^{-1}\widetilde{M}\mathbf{v} = \widetilde{\mathbf{F}}_2, \tag{4.2}$$

where $\widetilde{Q}$, $\widetilde{M}$, $\widetilde{\mathbf{F}}_1$ and $\widetilde{\mathbf{F}}_2$ include the SAT boundary treatment. The unknowns $\mathbf{v}_i$ are distributed on a primal grid x_i, and around each unknown there is a control volume Ω_i, where the flux points $x_{i\pm1/2}$ make the dual grid, see Figure 4.1. The matrices P and $\widetilde{M}$ depend on the dual and primal grid, respectively.

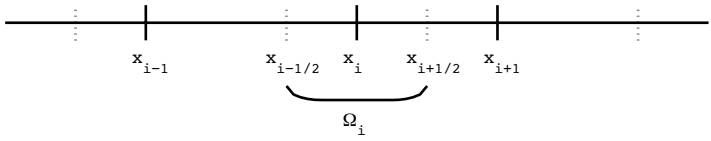

Figure 4.1. The control volume $\Omega_i = x_{i+1/2} - x_{i-1/2}$ on an unstructured mesh.

The truncation errors $\mathbf{T}_e$ are obtained by inserting the representation of the exact solution, $\mathbf{u}$, into the schemes (4.2). For an equidistant mesh the truncation error is second order accurate ($\mathbf{T}_e \sim h^2$) in the interior. For a random mesh, the truncation error can be as bad as zeroth order accurate ($\mathbf{T}_e \sim 1$). However, in practice it is the error of the solution, $\mathbf{e} = \mathbf{u} - \mathbf{v}$, which is relevant. The relations between the solution error and the truncation error are given by

$$P^{-1}\widetilde{Q}\mathbf{e} = \mathbf{T}_e, \qquad -P^{-1}\widetilde{M}\mathbf{e} = \mathbf{T}_e.$$

Usually the error $\mathbf{e}$ can only be described as a function of $\mathbf{T}_e$ in terms of estimates, with the typical conclusion that $\mathbf{e} \sim 1$ for a bad mesh. Nevertheless, better convergence rates have been observed in numerical simulations.

For these problems we have been able to compute the errors exactly by inverting the matrices $\widetilde{Q}$ and $\widetilde{M}$ analytically. It is found that the error contributions from the primal and the dual grid can be treated separately. The errors introduced by random perturbations of the mesh are analyzed using probability theory, and we show that in the hyperbolic case the errors are of order 0.5, that is $\mathbf{e} \sim \sqrt{h}$, for the worst mesh. The results from the analysis agree with the ones from numerical experiments.

Even though $\mathbf{e} \sim \sqrt{h}$ is a better result than $\mathbf{e} \sim 1$, the grid design is clearly very important for the end result. Especially for the hyperbolic problem, where the order of accuracy of the solution varied between 0.5 and 2, depending on the type of mesh. For the elliptic problem it varied between 1.5 and 2. It should also be noted that for the random meshes the results are *averages*, i.e. in a single simulation the method could do much worse (or better).

Contributions: The ideas were developed in close collaboration between the authors. The author of this thesis performed the analysis and the computations and wrote the manuscript.

4.2 Paper II

J. Nordström and S. Eriksson, Fluid structure interaction problems: the necessity of a well posed, stable and accurate formulation, Communications in Computational Physics, 8(5):1111–1138, 2010.

We study a fluid structure interaction (FSI) problem, arising from applications in for example aerodynamics or in medicine. The focus lies on the coupling conditions between the fluid and the structure, both for the continuous and the discretized problem. As our flow model we use the linearized Euler equations in one dimension,

$$U_t + AU_x = 0, \qquad 0 \le x \le x_1(t) \approx 1,$$

where the matrix A depends on the fluid, and the components of U are density ρ, velocity u, and temperature T. From this, the equation of state yields the pressure p. The right boundary is the time-dependent position of the structure, here modeled by a spring. The spring equation is

$$m\ddot{\Delta x} + b\dot{\Delta x} + k\Delta x = f,$$

where $\Delta x = x_1(t) - 1$ is the deviation from the equilibrium state, and f is the force acting on the spring. The constants m, k, b determine the spring properties. The computational domain $x \in [0,\ x_1(t)]$ depends on the solution, and this causes non-linearities in the problem. We study both the original non-linear problem and a linearized version of the problem. The coupling conditions between the fluid and the spring are derived for the linear problem. Using physical arguments as, (i) the flow should have the same velocity as the spring, and (ii) the force acting on the spring should be the pressure of the flow (in one dimension pressure and force is equal), the coupling conditions

become

$$u(1,t) = \dot{x}_1, \qquad f = p(1,t). \tag{4.3}$$

These conditions are confirmed by an unbiased mathematical derivation, demanding only well-posedness. We discretize the coupled system and use the SBP-SAT framework for deriving a stable numerical scheme. For the non-linear version of the problem we neither achieve well-posedness nor a stable scheme.

The eigenfrequencies of the linear continuous problem are computed using the Laplace transform technique. By giving the spring an initial displacement and studying the response from the system, we see that the eigenfrequencies of the numerical solution converge to the continuous ones as the mesh is refined.

An important aspect of FSI in aerodynamics is a phenomenon called flutter. It occurs when the wind varies at the eigenfrequency of the object, which will make the object oscillate with increasing amplitude. This is a very dangerous scenario and therefore it is of utmost interest to know the eigenfrequencies.

The following observations were made in the numerical experiments. To correctly detect the eigenfrequencies, high accuracy is necessary. A low order scheme or insufficient resolution will not yield good approximations of the eigenfrequencies. To stress the importance of having a stable numerical method, we compared the SAT coupling procedure to the injection method, which in some cases led to spurious instabilities. In addition, simulations using the non-linear scheme were performed (with the SAT boundary technique). However, the lack of well-posedness sometimes led to instabilities in this case as well. In both these cases, whether caused by lack of well-posedness or stability, the instabilities could be mistaken for flutter.

Contributions: The ideas were developed in close collaboration between the authors. The author of this thesis performed parts of the analysis and all the computations. The manuscript was written in close cooperation between the authors.

4.3 Paper III

S. Eriksson, Q. Abbas, and J. Nordström, A stable and conservative method for locally adapting the design order of finite difference schemes, Journal of Computational Physics, 230(11):4216–4231, 2011.

In this paper we construct a scheme that has different order of accuracy in different parts of the computational domain. For the derivation, we consider the advection equation $u_t + au_x = 0$, on the domain $x \in [-1,\ 1]$. At $x = 0$ we intend to shift the order of the scheme. Numerically this is approximated by

$$\mathbf{v}_t^L + aP_L^{-1}Q_L\mathbf{v}^L = \tau_L P_L^{-1} e_N(\mathbf{v}_N^L - \mathbf{v}_0^R), \quad \mathbf{v}_t^R + aP_R^{-1}Q_R\mathbf{v}^R = \tau_R P_R^{-1} e_0(\mathbf{v}_0^R - \mathbf{v}_N^L),$$

where $\mathbf{v}^L$ and $\mathbf{v}^R$ are the solutions in the left and right domain, respectively. $P_{L,R}$ and $Q_{L,R}$ are SBP operators, and $\tau_{L,R}$ are chosen such that the coupled equations are stable. At $x = 0$ there is a SAT interface, and both $\mathbf{v}_N^L$ and $\mathbf{v}_0^R$ are approximations of $u(0,t)$.

Our aim is to be able to move the interface, but the double solution values make that difficult. Under the assumption $\mathbf{v}_N^L = \mathbf{v}_0^R$ we modify the old scheme, and arrive at

$$\mathbf{W}_t + a\widetilde{P}^{-1}\widetilde{Q}\mathbf{W} = 0. \tag{4.4}$$

The operators $\widetilde{P}$ and $\widetilde{Q}$ in (4.4) are constructed by merging the original operators $P_{L,R}$, $Q_{L,R}$, as $\widetilde{P} = \mathrm{diag}(P_L^{0,0}, \ldots, P_L^{N-1,N-1},\ P_L^{N,N} + P_R^{0,0},\ P_R^{1,1}, \ldots, P_R^{N,N})$ and

$$\widetilde{Q} = \begin{bmatrix} Q_L^{0,0} & \cdots & Q_L^{0,N-1} & Q_L^{0,N} & & & \\ \vdots & \ddots & \vdots & \vdots & & & \\ Q_L^{N-1,0} & \cdots & Q_L^{N-1,N-1} & Q_L^{N-1,N} & & & \\ Q_L^{N,0} & \cdots & Q_L^{N,N-1} & Q_L^{N,N} + Q_R^{0,0} & Q_R^{0,1} & \cdots & Q_R^{0,N} \\ & & & Q_R^{1,0} & Q_R^{1,1} & \cdots & Q_R^{1,N} \\ & & & \vdots & \vdots & \ddots & \vdots \\ & & & Q_R^{N,0} & Q_R^{N,1} & \cdots & Q_R^{N,N} \end{bmatrix}.$$

The transformed scheme is thus smaller than the original system, and the solution vector $\mathbf{W}$ is one element shorter than the original total solution vector $\mathbf{V} = [\mathbf{v}_L^T, \mathbf{v}_R^T]^T$. The value $u(0,t)$ is now approximated by only *one* element in the vector $\mathbf{W}$.

The new scheme (4.4) possesses the SBP properties, i.e. $\widetilde{P} = \widetilde{P}^T > 0$ and $\widetilde{Q}$ is skew-symmetric in the interior (because $Q_L^{N,N} + Q_R^{0,0} = 0$). This automatically leads to a conservative and stable scheme. By modifying $\widetilde{Q}$ and $\widetilde{P}$ the scheme can be designed to switch order several times, instead of just once.

Numerical simulations are performed. In one case a propagating pulse is followed by a high order accurate discretization, while having second order accuracy away from the pulse. In addition, shock calculations are performed. When computing flows that have shocks, we use the MUSCL scheme. It is an established method that senses where the shock is and decreases the order from second to first. In the simulations we couple our adapting accuracy scheme to the MUSCL scheme and are thereby capable of following a shock with the low order stencil, and still have high order accuracy in the rest of the computational domain.

Contributions: The author of this thesis derived the new operators and did some of the numerical simulations. The computations using the MUSCL hybrid scheme were performed by the second author. The manuscript was written by the author of this thesis.

4.4 Paper IV

J. Nordström, S. Eriksson, and P. Eliasson, Weak and strong wall boundary procedures and convergence to steady-state of the Navier–Stokes equations, Journal of Computational Physics, 231(14):4867–4884, 2012.

In this paper we study how the choice of boundary implementation affects the convergence to steady-state. The problem considered is the Navier–Stokes equations with solid wall boundaries, where the boundary conditions are imposed either using a weak formulation (SAT), a strong formulation (injection), or a mixture of the weak and

strong formulations. First the theory for a general steady-state problem is described. Consider

$$\begin{aligned} U_t + \mathscr{A}U &= 0, \qquad x \geq 0, \qquad t \geq 0, \\ LU(0,t) &= 0, \\ U(x,0) &= f(x), \end{aligned}$$

where the ambition is to reduce U (defined as the deviation of the unsteady solution from the steady-state solution) from the initial data f and reach zero fast. Using the Laplace transform method we find that asymptotically $U(x,t) \sim e^{\eta^* t}$, and we denote η^* the continuous decay rate. If η^* is negative and large, the solution converges to zero fast. The semi-discrete version of the continuous problem is written

$$\begin{aligned} \mathbf{V}_t + \bar{A}\mathbf{V} &= 0, \qquad t \geq 0, \\ \mathbf{V}(0) &= \mathbf{f}, \end{aligned}$$

where $\mathbf{V}$ is the discrete approximation of U. The matrix $\bar{A}$ is the discrete version of $\mathscr{A}$, including the numerical implementation of the boundary conditions $LU = 0$. The sign and size of the real part of the eigenvalues λ_i of $\bar{A}$ are the crucial factors for obtaining steady-state solutions $\mathbf{V} = 0$. The discrete problem converges to steady-state if all $\mathrm{Re}(\lambda_i) > 0$. We denote $\min_i \mathrm{Re}(\lambda_i)$ the discrete decay rate. If $\min_i \mathrm{Re}(\lambda_i)$ is large, the convergence will be fast. To manipulate the eigenvalues of $\bar{A}$ directly is almost impossible, but we can guarantee convergence to steady-state if we have an energy stable numerical scheme. Therefore we examine the possibility that a stable (slightly dissipative) boundary treatment can modify $\bar{A}$ and affect the convergence rate.

In the analysis part of the paper we consider the constant coefficient version of the Navier–Stokes equations. We prove stability for the weak and the mixed schemes using the energy method. No proof is obtained for the strong formulation. The discrete decay rate is computed for the three different boundary procedures, and the weak scheme leads to faster convergence to steady-state than the other two schemes. The difference is most pronounced for coarse meshes. For fine meshes the discrete decay rates converges to the continuous decay rate for all three boundary procedures.

Numerical calculations using a flow solver for unstructured grids, EDGE, indicate that the linear results carry over to the fully nonlinear Navier–Stokes equations. In all simulations we tried, the solution from the weak scheme converged fast, which is consistent with the linear analysis. The solutions obtained by the mixed and strong schemes either converged slower or, in some cases, did not converge at all.

Contributions: The manuscript was written in close cooperation with the first author. The theory and computations of the linearized problem were performed by the author of this thesis. The EDGE computations were performed by the third author.

4.5 Paper V

S. Eriksson and J. Nordström, Exact non-reflecting boundary conditions revisited: well-posedness and stability, Technical report 2012-032, Department of Information Technology, Uppsala University, 2012.

In many aerodynamic applications, the flow field close to an aircraft (or other object) is studied. When performing numerical simulations it is not feasible to take the entire atmosphere into consideration, and at some distance away from the area of interest the computational domain is truncated by introducing artificial boundary conditions (ABCs). If this is not done with care, waves coming from the object will reflect back from the ABC and pollute the numerical solution.

We study a problem on the form (3.1), with

$$U = \begin{bmatrix} p \\ u \end{bmatrix}, \qquad A = \begin{bmatrix} v & c \\ c & v \end{bmatrix}, \qquad B = \begin{bmatrix} 0 & 0 \\ 0 & \varepsilon \end{bmatrix}, \qquad v > 0.$$

The singular B makes this an incompletely parabolic system of PDEs, which in many aspects makes it similar to the Navier–Stokes equations. We derive exact non-reflecting boundary conditions (NRBCs) for the Laplace transformed problem, (3.2), resulting in boundary conditions on the form

$$\begin{aligned} \hat{L}_L \hat{U} = \hat{g}_L \quad &\Longleftrightarrow \quad \begin{bmatrix} \alpha_1 & \beta_1 \\ \alpha_2 & \beta_2 \end{bmatrix} \begin{bmatrix} \hat{p} \\ \hat{u} \end{bmatrix} + \begin{bmatrix} 0 & \varepsilon \\ 0 & \varepsilon \end{bmatrix} \begin{bmatrix} \hat{p}_x \\ \hat{u}_x \end{bmatrix} = \begin{bmatrix} \hat{g}_1 \\ \hat{g}_2 \end{bmatrix}, \\ \hat{L}_R \hat{U} = \hat{g}_R \quad &\Longleftrightarrow \quad \begin{bmatrix} \alpha_3 & \beta_3 \end{bmatrix} \begin{bmatrix} \hat{p} \\ \hat{u} \end{bmatrix} + \begin{bmatrix} 0 & \varepsilon \end{bmatrix} \begin{bmatrix} \hat{p}_x \\ \hat{u}_x \end{bmatrix} = \begin{bmatrix} \hat{g}_3 \end{bmatrix}, \end{aligned}$$

where α_j and β_j depend on the time-dual variable s. Using the Laplace transform method we show that the NRBCs yield a well-posed problem in the GKS sense. This is followed by a derivation using the energy method, resulting in an energy estimate of the continuous solution.

The IBVP (3.1) is discretized in space using the SBP-SAT methodology, and the derivation of the SAT parameters is described in detail. By choosing the parameters in a suitable manner, and using the results from the continuous estimate, we are able to obtain an energy estimate of the discrete solution as well.

The NRBCs are derived in the Laplace transformed space, and when transformed back to the time domain, the SAT terms consist of convolutions. In the numerical implementation these are approximated using convolution quadratures. Numerical simulations are performed, showing that the solutions converge to the exact solution as the grid is refined. The exact NRBCs are compared with approximate NRBCs and Dirichlet boundary conditions. The exact NRBCs outperform the approximate NRBCs and the Dirichlet boundary conditions in all aspects.

Contributions: The manuscript was written by the author of this thesis. The derivations and numerical simulations were performed by the author of this thesis.

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6. Summary in Swedish

Stabila numeriska metoder med rand- och kopplingsvillkor för tillämpningar inom aerodynamik

Den här avhandlingen handlar om numeriska metoder för att lösa partiella differentialekvationer. Metoderna fungerar för många slags problem, men speciellt är det tillämpningar inom aerodynamik som avses. Problem inom aerodynamik innebär många utmaningar för den numeriska beräkningsmetod som används. Några av dessa tas upp och undersöks i den här avhandlingen, som luftens interaktion med en kropp (t.ex. ett flygplan), behandling av flödesproblem där det förekommer stötar och hur man kan hantera randvillkor. Dessa problem måste lösas på ett sätt som gör att den numeriska metoden förblir effektiv, noggrann och stabil.

För att lösningen till en partiell differentialekvation ska kunna bestämmas unikt krävs initial- och randvillkor, vilket leder till ett så kallat inital- och randvärdesproblem. För att få ökad förståelse studerar vi numeriska lösningar till inital- och randvärdesproblem som beskriver förenklade modellproblem inom aerodynamik. Dessa problem diskretiseras genom att använda noggranna finita differensscheman på partiell summationsform, eller SBP-form (eng. summation by parts), kombinerat med en svag randbehandling kallad SAT (eng. simultaneous approximation term). Med den här metodiken kan man härleda energiuppskattningar av lösningen, så att man kan garantera stabilitet. Huvudfokus för den här avhandlingen är implementeringen av rand- och kopplingsvillkor.

Den svaga randbehandlingen jämförs med en mer allmänt använd metod, injektionsmetoden, också kallad stark randbehandling. Analysen görs för de linjäriserade Navier-Stokes-ekvationerna, med fasta väggrandvillkor. Dessa randvillkor implementeras antingen svagt, starkt eller blandat starkt-svagt. För det svaga och blandade fallet kan vi bevisa att randbehandlingen leder till stabilitet, medan vi inte finner någon energiuppskattning i det starka fallet. Den svaga implementeringen av randvillkor gör att man kan öka hastigheten med vilken en lösning konvergerar mot den stationära lösningen. Beräkningar på de fullt olinjära Navier-Stokes-ekvationerna stödjer resultaten.

En annan aspekt av implementeringen av randvillkor uppkommer när man tittar på problem av fluid-struktur-interaktionstyp, det vill säga ett kopplat system av till exempel luft och ett flygplan. De här systemen har resonansfrekvenser, och om de utsätts för yttre påverkan i en sådan frekvens kan de börja vibrera med allt större utslag (självsvängning eller fladder). Detta fenomen kan vara oerhört farligt, och det är därför viktigt att korrekt kunna identifiera dessa frekvenser. Vi jämför en bevisbart stabil randbehandling med randimplementeringar där vi inte kunnat hitta en energiuppskattning. De numeriska resultaten visar att om inte randvillkoren implementeras på ett

stabilt sätt kan den numeriska lösningen uppvisa ett beteende som lätt går att missta för självsvängning.

För flödesproblem beskrivna av ickelinjära ekvationer kan diskontinuerliga lösningar, så kallade stötar, bildas. Vid en stöt bör det numeriska schemat ha första ordningens noggrannhet, annars uppstår ofta ofysikaliska oscillationer i den numeriska lösningen. Baserat på ett kopplat SBP-SAT-schema härleder vi ett konservativt och stabilt schema, där noggrannhetsordningen kan sänkas lokalt. Den nya metoden kopplas till en befintlig stöthanterande metod, MUSCL, vilken detekterar stötar och sänker noggrannheten från andra ordningens noggrannhet till första ordningens noggrannhet. På det här sättet skapas en hybridmetod som har låg noggrannhet nära stötar men behåller den höga noggrannhetsordningen i områden där lösningen är kontinuerlig. Till skillnad från det ursprungliga SBP-SAT-schemat är det lätt att under simuleringens gång ändra var schemat byter noggrannhet, vilket gör det möjligt att följa en propagerande stöt.

Vid tillämpningar där geometrin är komplicerad, är en lösning att koppla de noggranna finita differensmetoderna till en finit volymsmetod, eftersom den senare inte förutsätter strukturerade nät. Problemet är att noggrannheten hos finita volymsmetoderna kan vara svårgenomskådad. Trunkeringsfelet antyder nämligen att lösningen inte ens borde vara konsistent, medan numeriska experiment har påvisat åtminstone låg konvergensordning. Vi har undersökt hur noggrann lösningen blir om finita volymsmetoden används på ett ostrukturerat nät. Genom att härleda ett exakt uttryck för diskretiseringsfelen, och använda sannolikhetsteori för att hantera ickedeterministiskt genererade nät, kan vi visa att i värsta fall blir lösningen i snitt noggrann av ordning 0,5 för hyperboliska problem, och av ordning 1,5 för elliptiska problem.

Vi har också studerat artificiella randvillkor för domäner utan naturliga ränder. Exakta icke-reflekterande randvillkor härleds för ett Navier-Stokes-liknande linjärt system av partiella differentialekvationer, och vi visar att dessa randvillkor leder till välställdhet och en energiuppskattning av den kontinuerliga lösningen. Som en följd av detta blir även den numeriska approximationen stabil, eftersom vi använder ramverket SBP-SAT. Härledningen av randvillkoren och energiuppskattningarna, både i det kontinuerliga och i det diskreta fallet, görs i Laplace-transforms-rummet. Randvillkoren transformeras sedan tillbaka till tidsdomänen, och numeriska simuleringar utförs. De exakta icke-reflekterande randvillkoren jämförs med approximativa icke-reflekterande randvillkor och Dirichlet-randvillkor, och de exakta icke-reflekterande randvillkoren överträffar de båda andra i noggrannhet.

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