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# High Order Finite Difference Methods in Space and Time

BY

WENDY KRESS



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#### Abstract

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In this thesis, high order accurate discretization schemes for partial differential equations are investigated.

In the first paper, the linearized two-dimensional Navier-Stokes equations are considered. A special formulation of the boundary conditions is used and estimates for the solution to the continuous problem in terms of the boundary conditions are derived using a normal mode analysis. Similar estimates are achieved for the discretized equations. For the discretization, a second order finite difference scheme on a staggered mesh is used. In Paper II, the analysis for the second order scheme is used to develop a fourth order scheme for the fully nonlinear Navier-Stokes equations. The fully nonlinear incompressible Navier-Stokes equations in two space dimensions are considered on an orthogonal curvilinear grid. Numerical tests are performed with a fourth order accurate Padé type spatial finite difference scheme and a semi-implicit BDF2 scheme in time.

In Papers III-V, a class of high order accurate time-discretization schemes based on the deferred correction principle is investigated. The deferred correction principle is based on iteratively eliminating lower order terms in the local truncation error, using previously calculated solutions, in each iteration obtaining more accurate solutions. It is proven that the schemes are unconditionally stable and stability estimates are given using the energy method. Error estimates and smoothness requirements are derived. Special attention is given to the implementation of the boundary conditions for PDE. The scheme is applied to a series of numerical problems, confirming the theoretical results.

In the sixth paper, a time-compact fourth order accurate time discretization for the oneand two-dimensional wave equation is considered. Unconditional stability is established and fourth order accuracy is numerically verified. The scheme is applied to a two-dimensional wave propagation problem with discontinuous coefficients.

Keywords: finite difference methods, Navier-Stokes equations, high order time discretization, deferred correction, stability

Wendy Kress, Department of Information Technology, Scientific Computing. Uppsala University. Box 337, SE-751 05 Uppsala, Sweden

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"Obvious" is the most dangerous word in mathematics.

E. T. Bell (1883 - 1960)

The thesis is based on the following papers, which will be referred to in the text by Roman numerals I-VI

- [I] W. Kress and J. Nilsson, Boundary Conditions and Estimates for the Linearized Navier-Stokes Equations on Staggered Grids, Comp. & Fluids, 32 (2003), pp. 1093–1112.<sup>1</sup>
- [II] A. BRÜGER AND J. NILSSON AND W. KRESS, A Compact Higher Order Finite Difference Method for the Incompressible Navier-Stokes Equations, J. Sci. Comput., 17 (2002), pp. 551–560.<sup>2</sup>
- [III] B. GUSTAFSSON AND W. KRESS, *Deferred Correction Methods for Initial Value Problems*, BIT, 41(5) (2001), pp. 986–995.<sup>3</sup>
- [IV] W. KRESS, B. GUSTAFSSON, Deferred Correction Methods for Initial Boundary Value Problems, J. Sci. Comp., 17 (2002), pp. 241–251. <sup>4</sup>
- [V] W. KRESS, Error Estimates for Deferred Correction Methods in Time, IT Scientific Report 2003-040, ISSN 1404-3203, Department of Information Technology, Uppsala University, August 2003. Downloadable from Web site http://www.it.uu.se/research/reports. Submitted to SIAM J. Numer. Anal.
- [VI] W. KRESS, A Compact Fourth Order Time Discretization Method for the Wave Equation, IT Scientific Report 2003-041, ISSN 1404-3203, Department of Information Technology, Uppsala University, August 2003. Downloadable from Web site http://www.it.uu.se/research/reports.

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#### 1

#### Introduction

Differential equations describe processes in many scientific fields. Traditionally, they occur in physics and engineering. Lately, mathematical models leading to differential equations have been increasingly studied in other fields such as biology, medicine, chemistry, financial mathematics and even psychology.

For some of the equations, exact solutions can be calculated. Others are too complex to be solved exactly. There, numerical methods are used.

When considering numerical methods for the solution of a partial differential equation (PDE) or ordinary differential equation (ODE), a number of aspects have to be considered.

- The solution of the numerical scheme should be a good approximation to the exact solution.
- The numerical scheme should be efficient in that the computational cost and the memory requirements on a computer are within a reasonable limit.

An important aspect when studying differential equations and their numerical solution is wellposedness and stability. On the one hand the original problem and the associated numerical problem should be uniquely solvable when corresponding initial and boundary conditions are given. The solution should also depend continuously on the data, i.e., small changes in the initial and boundary data should result in small changes in the solution. For the numerical scheme, this is important to establish estimates for the error. Stability is also crucial for the performance of the scheme. Unstable schemes are practically useless in applications.

In the first part of this thesis, we consider a special set of differential equations, the incompressible Navier-Stokes equations. We consider a finite difference scheme for discretizing the equations and investigate the wellposedness of the equations and the stability of the scheme under a special set of boundary conditions.

In the second part, we consider time discretization schemes for general systems of PDEs and ODEs and their stability.

In both parts of the thesis, we investigate high order accurate schemes. High order accurate schemes have the advantage of admitting a coarser grid to reach

a certain accuracy. Common arguments against using high order schemes are that they tend to be more complicated to implement and more expensive to calculate than lower order schemes. High order time discretization schemes are often less stable. In this thesis, we consider high order discretizations that do not give rise to these kinds of problems. A compact fourth order accurate scheme in space is considered. In the second part of the thesis, we present high order accurate time discretizations that are unconditionally stable and the computational complexity is comparable to that of a second order method.

### Navier-Stokes equations

The dynamics of fluids and gases are governed by the Navier-Stokes equations which are derived from basic physical laws, the conservation of mass, momentum and energy. The derivation of the Navier-Stokes equations can be found in many textbooks, e.g., [1], [21] and [22], which are also a good introduction into the field of computational fluid dynamics. When making certain assumptions about the fluid (incompressible, non-heat conducting, viscous, homogeneous flow with no body forces), one obtains the *incompressible Navier-Stokes equations*,

$$\mathbf{u}_t + (\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p = \mathbf{v}\Delta \mathbf{u}, \nabla \cdot \mathbf{u} = 0,$$
 (2.1)

for the velocity vector  $\mathbf{u}$  and the kinematic pressure p. The quantity  $\mathbf{v}$  is the kinematic viscosity coefficient. The incompressibility assumption is valid for fluids. For gases, which are generally highly compressible, it is possible to show that the variation in the density is negligible at low Mach number flow, i.e., low velocities compared to the speed of sound. Thus, the use of the incompressible Navier-Stokes equations for low Mach number flow is justified. When formulating the Navier-Stokes equations, several different variants are used. The most direct formulation is the *primitive variable formulation* (2.1). The *vorticity-stream function formulation* introduces the vorticity  $\mathbf{\omega} = \nabla \times \mathbf{u}$  and the vector potential  $\mathbf{\psi}$  defined by  $\nabla \times \mathbf{\psi} = \mathbf{u}$ . Equations for  $\mathbf{\omega}$  and  $\mathbf{\psi}$  are derived from the original Navier-Stokes equations.

$$\omega_t + \nabla \times (\omega \times (\nabla \times \psi)) = \nu \Delta \omega,$$
  
$$\Delta \psi = -\omega.$$

The pressure has been completely eliminated from the equations. Another formulation is the *vorticity-velocity formulation*, using  $\omega$  and  $\mathbf{u}$ .

$$\mathbf{u}_t + \boldsymbol{\omega} \times \mathbf{u} + \nabla p_T = -\nu \nabla \times \boldsymbol{\omega},$$
  
$$\nabla \cdot \mathbf{u} = 0.$$

introducing the total pressure  $p_T = p + \frac{1}{2} |\mathbf{u}|^2$ . The vorticity-velocity formulation is of advantage for nearly irrotational flow since the first equation simplifies to approximately  $\mathbf{u}_t + \nabla p_T = 0$ . Another feature is the fact that only first order derivatives are present in the equations. This might simplify the discretization. A difficulty, when introducing the vorticity is the choice of boundary conditions that give rise to an equivalent system to the original Navier-Stokes equations. An overview over the different formulations is given in [11]. In the first part of this thesis, we consider the primitive variable formulation of the Navier-Stokes equation (2.1). Due to the lack of a time derivative for the pressure, some complications arise in the discretization and often, an alternative formulation is used. Taking the divergence of the first equation in (2.1) and using the continuity equation,  $\nabla \cdot \mathbf{u} = 0$ , one arrives at a Poisson equation for the pressure, which can be used instead of the original continuity equation. This is referred to as the pressure Poisson equation (PPE) formulation . Another way to overcome the lack of a time derivative for the pressure is the artificial compressibility formulation introduced in [4]. The modification of the equations is necessary for the direct implementation of explicit time integration methods, as there is no way of explicitly advancing the pressure in time in the original formulation. A problem with the alternative formulations (PPE and artificial compressibility) is to obtain correct boundary conditions for the pressure. In [35], an analysis of different boundary conditions for the pressure is performed. This issue is also addressed in [11], where the "correct" boundary conditions for the pressure are derived for some problems.

We will here discuss the Navier-Stokes equations in primitive variable formulation with the original continuity equation. We use a semi-implicit time integration, treating all linear terms implicit in time. This allows us to solve the equations directly without the use of a pressure Poisson equation or artificial compressibility.

#### 2.1 Spatial discretization

To solve the Navier-Stokes equations numerically, a large variety of techniques are in use. We here focus on finite difference methods. High order accurate methods in space are necessary when trying to solve problems with very small scales. In order to resolve a certain wavelength in space there is a minimum number of required points per wavelength (PPW). The required PPW for higher order methods are usually some factors lower than for a first or second order scheme. A recent paper examining this is [23]. For computations of realistic flow with small scale structures, the memory requirements for lower order methods will be extensive and the use of high order schemes is essential. The best resolution is of course achieved with spectral methods. These

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methods are, however, more difficult to apply for complicated geometries. A general complication when using higher order schemes is the treatment of the boundary conditions. The computational stencil becomes wider for higher order schemes, and numerical boundary conditions have to be introduced. It is not trivial how to choose numerical boundary conditions, to retain the stability of the scheme [3]. Another matter is the fact that using higher order schemes leads to an increase in the amount of work per grid point in time, especially when using implicit time-marching schemes. The number of grid points in time can, however, often be dramatically reduced for higher order schemes. In addition, there exist methods, for which the amount of work and the stencil size will not be very much higher. One such example are compact schemes of  $Pad\acute{e}\ type$ . The fourth order Padé type approximation for the first derivative of a function f(x) is given by

$$\frac{1}{6}f'(x-h) + \frac{2}{3}f'(x) + \frac{1}{6}f'(x+h) = \frac{1}{2h}(f(x+h) - f(x-h)).$$

The stencil is similar to that of a centered second order scheme, with the difference that the derivative is solved for implicitly. To solve for f', a tridiagonal system needs to be solved, which can be done in a very efficient way.

A problem with some discretization schemes is the existence of spurious, oscillatory solutions. This can be remedied by using a *staggered grid*, i.e., the different components of the solution are stored at different points in space and sometimes even time. In addition to removing the oscillatory solutions, staggered grid schemes often add compactness to the stencil. In [42], a high order compact upwind scheme on a staggered mesh is used for the Navier-Stokes equations. Fourth and sixth order schemes on a regular grid have been considered e.g. in [20] and [37]. In [30], the conservation properties of some high order schemes are discussed and a fourth order conservative scheme is presented. Recently, conservative staggered grid approaches have been used on unstructured grids in [34]. In [27] and [28], a fourth order compact scheme is considered for the vorticity formulation. In [38], a comparison of several high order methods is done. Compact schemes for the velocity-vorticity formulation in two dimensions are discussed in [9] and in [29], a compact fourth order scheme in velocity-vorticity formulation for 3D flow is presented.

#### 2.2 Paper I

In order to guarantee the convergence of the discrete solution to the exact solution of the Navier-Stokes equations, the wellposedness of the continuous problem and the stability of the numerical scheme need to be established, i.e., we need to obtain an estimate of the solution in terms of the initial and bound-

ary data. One important aspect is the formulation and the discretization of the boundary conditions.

There are two important steps in the stability analysis. The first problem consists of establishing the stability of the corresponding Cauchy problem where the domain stretches over the entire space. For the discretization scheme, this will in general give conditions for the maximal permissible timestep. Under the assumption that the Cauchy problem is stable for a given timestep, one then considers the original initial boundary value problem with zero initial data and zero forcing function and studies the influence of the boundary conditions on the solution. The results of these two investigations can then be combined to an estimate for the solution of the original problem in terms of the initial and boundary data and forcing terms.

In Paper I, we consider the influence of the boundary conditions on the solution. A commonly used formulation of the boundary conditions is the prescription of the velocity components on the boundary and one condition for the pressure, either prescribing the pressure at one point in the domain, or prescribing the integral of the pressure over parts of the domain. The divergence equation will impose an additional restriction on the velocity on the boundary since

$$\int_{\partial\Omega} \mathbf{u} \cdot \mathbf{n} = -\int_{\Omega} \nabla \cdot \mathbf{u} = 0. \tag{2.2}$$

This condition is of course natural for the continuous problem. It is not straightforward how to transfer it to the discrete problem, and it is susceptible to perturbations in the sense that the system becomes unsolvable if condition (2.2) is slightly violated. In Paper I, we therefore consider an alternative way of formulating the boundary conditions.

The original Navier-Stokes equations are nonlinear. In order to perform an analysis, the problem is linearized by freezing the coefficients. We consider the linearized Navier-Stokes equations in two spatial dimensions with the velocity u and v in x and y-direction, respectively. We assume periodicity in one direction. With these assumptions, we arrive at the following problem in two space dimensions.

$$u_{t} + \bar{u}u_{x} + \bar{v}u_{y} + p_{x} = v(u_{xx} + u_{yy}),$$
  

$$v_{t} + \bar{u}v_{x} + \bar{v}v_{y} + p_{y} = v(v_{xx} + v_{yy}),$$
  

$$u_{x} + v_{y} = 0,$$
(2.3)

with constants  $\bar{u}$  and  $\bar{v}$ . We investigate the wellposedness of the system for

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boundary conditions of the form

$$u(t,0,y) - \frac{1}{2\pi} \int_0^{2\pi} u(t,0,y) dy = w_0(t,y), \text{ with } \int_0^{2\pi} w_0(t,y) dy = 0,$$

$$u(t,1,y) = u_1(t,y), \quad v(t,0,y) = v_0(t,y), \quad v(t,1,y) = v_1(t,y), \quad (2.4)$$

$$\int_0^{2\pi} p(t,0,y) dy = q_0(t),$$

and periodicity conditions in the *y*-direction. Now, (2.2) is not affected by the boundary conditions. The boundary conditions are such that small perturbations in (2.4) will still render a solvable set of equations. We refer to [14] for details, where a corresponding analysis has been done for the steady state Stokes equations. With the periodicity assumption, one can use a Fourier transform in the *y*-direction and a Laplace transformation in time, to write the general solution in the following form

$$(u,v,p)^T(t,x,y) = \int_{\eta-i\infty}^{\eta+i\infty} \sum_{\omega=-\infty}^{\infty} (\tilde{u},\tilde{v},\tilde{p})^T(s,x,\omega) e^{i\omega y + st} ds \quad \eta > 0.$$

Applying this to the differential equation, one is left with a system of ordinary differential algebraic equations (DAE) for  $(\tilde{u}, \tilde{v}, \tilde{p})$ . A general solution in terms of the transformation variables  $\omega$  and s has the form

$$(\tilde{u}, \tilde{v}, \tilde{p})^T(s, x, \omega) = a_{\omega}^s \mathbf{f}_1(s, x, \omega) + b_{\omega}^s \mathbf{f}_2(s, x, \omega) + c_{\omega}^s \mathbf{f}_3(s, x, \omega) + d_{\omega}^s \mathbf{f}_4(s, x, \omega).$$

There are four undetermined coefficients  $(a_{\omega}^s, b_{\omega}^s, c_{\omega}^s, d_{\omega}^s)$  in the general solution. They will be determined by the four boundary conditions. The next step is to find an estimate of the solution in terms of the boundary data. It turns out that the dependence of the undetermined coefficients on the boundary data can be expressed as

$$A^s_\omega \left(egin{array}{c} a^s_\omega \ b^s_\omega \ c^s_\omega \ d^s_\omega \end{array}
ight) = \left(egin{array}{c} ilde{w}_0 \ ilde{u}_1 \ ilde{v}_0 \ ilde{v}_1 \end{array}
ight),$$

where  $(\tilde{w}_0, \tilde{u}_1, \tilde{v}_0, \tilde{v}_1)^T$  are Fourier-Laplace transformations of the boundary data and  $A^s_\omega$  is a four by four matrix, depending on  $\omega$  and s. For wellposedness of the Fourier-Laplace transformed system of DAE, we need a uniform bound on the matrix  $A^s_\omega$  and uniform boundedness away from zero for the determinant  $\det(A^s_\omega)$  for all  $\omega$  and s. This will render boundedness of the undetermined coefficients  $(a^s_\omega, b^s_\omega, c^s_\omega, d^s_\omega)$ . If in addition the functions  $\mathbf{f}_i$  are uniformly bounded, we can derive an estimate of the solution  $(\tilde{u}, \tilde{v}, \tilde{p})^T(s, x, \omega)$  in terms of the boundary data. By Parseval's identity, a corresponding estimate follows for (u, v, p).

The main result for the continuous problem is the following.

**Conjecture 1.** Assume that the boundary data  $w_0$ ,  $u_1$ ,  $v_0$ ,  $v_1$  are  $2\pi$ -periodic in y and  $\int_0^{2\pi} w_0(t,y) dy = 0$ , but otherwise arbitrary. Then the system (2.3) with boundary conditions (2.4) and zero initial conditions has a unique solution, and there is an estimate

$$\int_{0}^{\infty} e^{-2\eta t} \|\mathbf{v}(t,\cdot,\cdot)\|^{2} dt \leq const \left( \int_{0}^{\infty} e^{-2\eta t} \left( \|q_{0}(t)\|^{2} + \|\mathbf{v}_{B}(t,\cdot)\|^{2} \right) dt \right),$$

$$\int_{0}^{\infty} e^{-2\eta t} \|p(t,\cdot,\cdot)\|^{2} dt \leq const \left( \int_{0}^{\infty} e^{-2\eta t} \left( \|q_{0}(t)\|^{2} + \|\mathbf{v}_{B}(t,\cdot)\|^{2} \right) dt \right),$$

$$+ \left\| \frac{\partial \mathbf{v}_{B}}{\partial y}(t,\cdot) \right\|^{2} + \left\| \frac{\partial \mathbf{v}_{B}}{\partial t}(t,\cdot) \right\|^{2} dt \right),$$

$$\forall \eta > 0.$$

Here, 
$$\mathbf{v} = (u, v)^T$$
 and  $\mathbf{v}_B = (w_0, u_1, v_0, v_1)^T$ .

In the proof, we numerically establish the boundedness away from zero of the determinant of the matrix  $A_{\omega}^{s}$ . Together with the boundedness of the matrix elements and the functions  $\mathbf{f}_{i}$ , we obtain an estimate of the solution in Fourier-Laplace space.

We now turn to the discretization of (2.3) and (2.4). To discretize the problem, a second order finite difference scheme on a staggered grid in space is used together with a semi-implicit version of the BDF2 scheme in time. The study of a second order scheme serves as a basis for the fourth order scheme used later on. The reason for using a semi-implicit discretization in time is that when later considering the fully nonlinear Navier-Stokes equations, it is practical to treat the nonlinear terms explicitly in time, whereas the linear terms can be treated implicitly. The integrals in (2.4) are replaced by summation and  $w_0$  is chosen such that  $\sum_j w_0(t,y_j) = 0$ . In order to obtain stability estimates for the discrete solution, we follow the procedure for the continuous problem. We find an estimate of the discrete solution in terms of the boundary data, now using a discrete Fourier transform in the y-direction and a discrete Laplace transform (z transform) in time.

Numerical experiments performed on a rectangular domain verify the second order accuracy of the scheme. In the experiments, problems with periodic solutions in y as well as nonperiodic problems are considered. In addition to problems with constant coefficients, an example with  $\bar{u}$  and  $\bar{v}$  being functions of time and space is studied. Also here, second order accuracy is obtained.

#### 2.3 Paper II

The analysis in Paper I has shown that the chosen boundary conditions lead to wellposed problems both for the continuous linearized Navier-Stokes equa-

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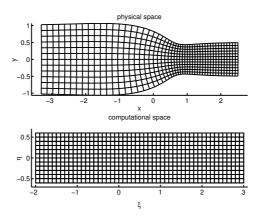


Figure 2.1: Transformation between the physical and computational space.

tions and a second order discretization. We now use these boundary conditions for the two-dimensional nonlinear Navier-Stokes equations and a fourth order discretization in space. A stability analysis for the scheme used here has been done in [12] for periodic boundary conditions.

As discussed in the introduction, it is desirable to use higher order methods to decrease the number of necessary grid points for the numerical simulation of turbulent flow, which is characterized, among other properties, by small scale structures.

Here, a fourth order Padé type scheme on a curvilinear orthogonal grid is used. The Padé scheme in its original formulation is applicable to a uniform equidistant cartesian grid. A discussion of the scheme on an equidistant grid can be found in [15]. To apply the scheme to an orthogonal curvilinear grid, we use a transformation from the physical space (x,y) to a uniform equidistant cartesian grid in the computational space  $(\xi,\eta)$ , see Figure 2.1. Formulating the Navier-Stokes equations in the new coordinate system  $(\xi,\eta)$  will lead to equations for the pressure and the new velocity components in the  $\xi$  and  $\eta$  direction, respectively. These equations are then solved on a cartesian equidistant grid.

Experimental results for a test problem on a ring shaped domain using polar coordinates and results for a laminar flow in a constricting channel are presented. For the experiment on the ring, we add a forcing term to the equations in order to be able to construct problems with a known exact solution. This allows us to examine the accuracy of the scheme. For the constricting channel problem, a numerical solution on a fine grid is used as a reference solution. The errors for the ring problem are very small and the order of accuracy is four and partly exceeds four. For the constricting channel problem, the accuracy order is higher than four for small Reynolds numbers (large viscosity coefficients v) and moderately deformed geometries. When increasing the Reynolds

number and considering sharper corners in the domain, the accuracy is slightly decreased.

#### Time discretization methods

We now turn to the time discretization of general PDEs. Many methods are based on the *method of lines*, i.e., the PDEs are first discretized in space, leading to a large system of ODEs or DAEs which can then be treated by any time stepping scheme for ODEs. A large amount of literature is available on the numerical treatment of ODEs. A survey of currently used methods can be found in [2]. Standard textbooks for numerical methods for ODEs are [18] and [19] and a recent textbook is [8]. We are interested in higher order accurate time discretization. In practice, first and second order accurate schemes are predominantly used, often due to the simpler form of the schemes or due to the fact that higher order schemes have a decreasing stability domain, leading to more severe time-step restrictions. Higher order schemes are, however, of advantage, especially in long term time integration. In this thesis, we consider two classes of stable high order schemes, deferred correction schemes and time compact schemes. They are easy to implement and the work per time-step is comparable to lower order methods. We first give a brief overview over some standard time-marching methods. We assume here that the method of lines is used and that the arising system is a linear system of ODEs, i.e., we consider a problem of the form

$$\frac{d}{dt}u(t) = A(t)u(t) + F(t) \text{ for } t \in (0,T),$$

$$u(0) = f.$$
(3.1)

Here,  $u(t), F(t), f \in \mathbf{R}^N$ , and  $A(t) \in \mathbf{R}^{N \times N}$ . The boundary conditions of the original PDE are assumed to be incorporated into the linear operator A(t) and the forcing term F(t). One can discretize (3.1), using any method available for the time integration of ODEs. One has to be careful, however, to choose a suitable method, in order to obtain satisfactory results. The resulting system of ODEs is usually very large. A realistic size of a problem in three space dimensions can be one million unknowns or more. Another matter is the stability of the scheme. A common way to analyze the stability for systems of ODEs is to simplify the analysis by considering a scalar ODE. If A(t) is uniformly diagonalizable, the system of equations can be decomposed into a set of

scalar equations. One obtains a stability bound in terms of the spectral radius of A(t). For nondiagonalizable matrices the simplification to scalar problems is not possible. The scalar stability analysis will, however, give a very good indication of the stability properties of the method even for systems of ODEs. In [24], a different definition of stability is considered for hyperbolic problems based on locally stable schemes and the resolvent condition from the stability theory for continuous PDEs. In [26], stability of some Runge-Kutta schemes is established by the energy method for systems with a coercive matrix. In the last four papers, we consider a stability analysis based on the energy method for semibounded matrices. From the stability analysis, one will usually obtain a condition on the maximal time-step depending on the spatial grid size. This is called the CFL condition. When using a small space-step, we have to match this with an often unnecessarily small time-step. This results in an enormous increase in work to solve the problem. In some cases it is of course necessary from accuracy considerations to choose the time-step in a certain way. However, the CFL condition will often give a very severe restriction that is not justified by the accuracy requirements. One way to avoid this problem is to use A-stable methods, which are stable independent of the size of the timestep. There are several theoretical results about A-stable methods, the most famous ones are probably the results by Dahlquist from 1963, see [6], stating that the order of an A-stable linear multistep method cannot exceed two (Second Dahlquist Barrier) and that an explicit linear multistep method cannot be A-stable.

Two classes of standard time discretization methods are linear multistep methods and Runge-Kutta schemes. The results by Dahlquist exclude linear multistep methods when requiring a high order A-stable method, leaving only implicit Runge-Kutta methods, and multistep Runge-Kutta methods. The Daniel-Moore Conjecture, see [7], [41], states that one can indeed construct A-stable Runge-Kutta methods of arbitrary order. The highest possible order of an A-stable j-stage Runge-Kutta multistep method is 2j. A fully implicit j-stage Runge-Kutta method involves the solution of an  $(N \cdot j) \times (N \cdot j)$  system per time-step. This can be extremely costly for large N. There are special classes of Runge-Kutta methods, diagonally implicit Runge-Kutta (DIRK) schemes, yielding a block lower triangular system to be solved, i.e., only the solution of  $j N \times N$  systems is required. The highest possible order of DIRK schemes is usually j. In order to obtain a method of order 2j, we need to solve  $2j N \times N$  systems for each time-step.

Another way of obtaining high order A-stable methods is Richardson extrapolation. This is based on combining the results of a lower order scheme on different meshes to a higher order approximation by cancelling terms in the global error expansion. To obtain a 2j-th order method, j solutions on different meshes are required when considering a symmetric second order accurate

base scheme.

In this thesis, we consider the deferred correction approach to obtain high order accurate stable schemes. We obtain a 2j-th order accurate scheme that will require the solution of  $j N \times N$  systems per time-step. Deferred correction has first been introduced by Fox [10] and a lot of work has been done by Pereyra in a series of papers starting with [33].

The deferred correction principle for general partial differential equations is as follows. Consider the general differential equation

$$\mathcal{L}u = f \text{ in } \Omega,$$

$$\mathcal{B}u = g \text{ on } \partial\Omega.$$

The operator  $\mathcal{L}$  is a linear differential operator and  $\mathcal{B}$  includes initial and boundary conditions. We consider an r-th order accurate discretization,

$$L_h u_h = f \text{ in } \Omega_h,$$
  
 $B_h u_h = g \text{ on } \partial \Omega_h.$ 

Assume for now that the initial and boundary conditions are fulfilled exactly, i.e.,  $B_h = \mathcal{B}|_{\partial\Omega_h}$ . Calculating an asymptotic expansion of the local truncation error, we obtain

$$L_h(u|_{\Omega_h})-f=\sum_{i=r}^{2r-1}h^i(\mathcal{D}_iu)|_{\Omega_h}+\mathcal{O}(h^{2r})\,,$$

where  $\mathcal{D}_i u$  are higher order differential operators. One now discretizes  $\mathcal{D}_i$  by difference operators  $D_{ih}$ . The deferred correction scheme is as follows

- Step 1: Solve  $L_h u_h = f$  with  $B_h u_h = g$ . Step 2: Solve  $L_h \tilde{u}_h = -\sum_{i=r}^{2r-1} h^i D_{ih} u_h + f$  with  $B_h \tilde{u}_h = g$ .

Under the assumption that  $\mathcal{D}_i$  are approximated to order r by  $D_{ih}$ , the scheme will formally be of order 2r. The process can be repeated to iteratively obtain arbitrarily high order approximations, gaining r orders of accuracy in each iteration step.

Different from Richardson extrapolation, only one mesh is needed for all intermediate solutions. Richardson extrapolation is based on an asymptotic expansion of the global error. In some cases, it is difficult to prove the existence of such an expansion, whereas we can directly calculate the local truncation error used in the deferred correction scheme.

When comparing the deferred correction to high order implicit Runge-Kutta schemes, the computational complexity is lower for the deferred correction the solution of an  $(N \cdot i) \times (N \cdot i)$  system per time-step for the Runge-Kutta scheme versus the solution of  $j N \times N$  systems for the deferred correction scheme.

#### 3.1 Paper III

The deferred correction principle has mainly been used to obtain high order accurate schemes in space. We here use it to obtain high order accurate time integration schemes.

In Paper III, we consider problem (3.1) for constant matrices A. The treatment of time-dependent A = A(t) is similar, although the stability analysis will become a bit more technical. The time-dependent case is treated in Papers IV and V. We use the concept of deferred correction to obtain high order accurate, stable schemes. As an underlying scheme, the implicit midpoint rule (IMR)<sup>1</sup> is used. It is second order accurate and A-stable. We introduce the notation

$$D_+ u^n = D_- u^{n+1} = \frac{u^{n+1} - u^n}{\Delta t}$$
,

$$E_+u^n=\frac{u^{n+1}+u^n}{2}.$$

The procedure described in the previous section can be used to obtain solutions of increasing order of accuracy, gaining two orders of accuracy in each step. The sixth order deferred correction scheme is as follows.

• Step 1: Solve

$$D_{+}u^{2,n} = AE_{+}u^{2,n} + F(t^{n+1/2}), \quad n = 0, ...,$$
  
 $u^{2,0} = f.$ 

• Step 2: Solve

$$D_{+}u^{4,n} = AE_{+}u^{4,n} + F(t^{n+1/2})$$

$$+ \frac{\Delta t^{2}}{24}D_{+}(D_{+}D_{-})u^{2,n}$$

$$- \frac{\Delta t^{2}}{8}AE_{+}(D_{+}D_{-})u^{2,n}, \quad n = 0, \dots,$$

$$u^{4,0} = f.$$

The value of  $u^{2,-1}$  is calculated by high order extrapolation from  $u^{2,n}$ ,  $n \ge 0$ .

<sup>&</sup>lt;sup>1</sup>In Paper III, the scheme is referred to as the trapezoidal rule, which is usually defined slightly differently. The notation has been changed to implicit midpoint rule in the following papers.

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• Step 3: Solve

$$\begin{split} D_{+}u^{6,n} &= AE_{+}u^{6,n} + F(t^{n+1/2}) \\ &+ \frac{\Delta t^{2}}{24}D_{+}(D_{+}D_{-})u^{4,n} \\ &- \frac{\Delta t^{2}}{8}AE_{+}(D_{+}D_{-})u^{4,n} \\ &- \frac{3\Delta t^{4}}{640}D_{+}(D_{+}D_{-})^{2}u^{4,n} \\ &+ \frac{3\Delta t^{4}}{128}AE_{+}(D_{+}D_{-})^{2}u^{4,n} , \quad n = 0, \dots, \end{split}$$

The values of  $u^{4,-1}, u^{4,-2}$  are calculated by high order extrapolation from  $u^{4,n}, n \ge 0$ .

Numerical test examples show a significant decrease of the error norms and the expected order of accuracy for a hyperbolic and a parabolic problem with periodic boundary conditions in space, Tables 3.1 and 3.2. There,  $u^p$  denotes the p-th order deferred correction solution,  $u^*$  denotes the exact solution, and the norm  $\|\cdot\|_h$  denotes the  $l^2$ -norm over space and time.

Table 3.1: Error for a parabolic equation.

М	20	40	80	order of accuracy
$  u^2 - u^*  _h$	2.4e-3	6.0e-4	1.5e-4	2.0
$  u^4 - u^*  _h$	1.0e-5	6.4e-7	4.0e-8	4.0
$  u^6 - u^*  _h$	1.0e-7	1.9e-9	3.2e-11	5.8

Table 3.2: Error for a hyperbolic equation.

М	20	40	80	order of accuracy
$  u^2 - u^*  _h$	1.8e-4	4.3e-5	1.1e-5	2.0
$  u^4 - u^*  _h$	2.6e-7	1.5e-8	9.3e-10	4.1
$  u^6 - u^*  _h$	1.5e-8	2.4e-10	3.6e-12	6.0

#### 3.2 Paper IV

As stated above, we are interested in schemes with no stability limitations on the time-step. We establish the unconditional stability of the deferred correction scheme under certain smoothness restrictions. We now consider time-dependent A(t). The stability estimate is obtained by using the energy method under the assumption that the matrix functions A(t) are semibounded, i.e.,

$$(u, A(t)u) \le 0 \quad \forall u \in \mathbf{R}^N, \text{ where } (u, v) = \frac{1}{N} \sum_{j=1}^N u_j v_j.$$

The main stability result is

**Theorem 1.** Assume that  $A(t_n)$  are semibounded matrices that commute with each other for all  $t_n = n\Delta t$ . Then the p-th order solution  $u^{p,n} \approx u(t_n)$  of the deferred correction algorithm satisfies the estimate

$$\|u^{p,n}\| \le const \left(\max_{0 \le \mu_i \le n-1+p(p-2)/8} \left\| \left(\prod_{i=1}^j A(t_{\mu_i+1/2})\right) f \right\| + \max_{0 \le \mu_i, \nu \le n-1+p(p-2)/8} \left\| \left(\prod_{i=1}^j A(t_{\mu_i+1/2})\right) F^{\nu+1/2} \right\| \right).$$

*Here, the constant depends on p and on t<sub>n</sub> but not on A*(t).

More general time-dependent A(t) are considered in Paper V. In the stability estimate, terms of the form  $A^jf$  and  $A^jF$  are present. This is different from the usual definition of stability, where the solution only depends on the initial data and the forcing terms. The interpretation of the above stability estimate for systems arising from PDEs is that if A is a discretized spatial operator, the action of A corresponds to a derivative in space, i.e., the estimate includes approximate spatial derivatives of the data. This is true for periodic problems. For problems which include boundary conditions, however, a deeper investigation has to be made. It turns out that the original boundary conditions will cause Au to be unbounded even for vectors u that are approximating smooth functions. When applying the deferred correction scheme to initial boundary value problems, oscillations occur at the boundary. There is, however, a way of formulating the boundary conditions to avoid these problems. In Paper V, a more thorough investigation is made.

Note that error bounds derived directly from this stability estimated by considering the difference equation for the error  $e^{2j,n} = u^{2j,n} - u(t_n)$  do not lead to higher order accuracy. The direct application of Theorem 1 on the error will actually only lead to second order accuracy results. To rigorously determine

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the order of accuracy of the scheme, a more elaborate analysis is necessary, which follows in Paper V.

Numerical experiments are performed for a hyperbolic, nonperiodic problem with time-dependent coefficients. Modified boundary conditions are used to ensure boundedness of the terms in the stability estimate. In addition, a system of parabolic PDEs with periodic boundary conditions is considered. Again, low errors and high order of accuracy are achieved.

#### 3.3 Paper V

In the two previous papers, the deferred correction scheme has been applied to the implicit midpoint rule. Another second order *A*-stable scheme that can be used is the implicit second order backward differentiation formula (BDF2),

$$\frac{3}{2}D_{+}u^{n} - \frac{1}{2}D_{-}u^{n} = Au^{n+1} + F^{n+1}.$$

The BDF2 scheme is dissipative. This will decrease the oscillations occurring at the boundary, when the original formulation of the boundary conditions are used. In addition, it turns out that the theoretical smoothness requirements can be relaxed by one power of A. The last property is due to the fact that no approximation of the right hand side of equation (3.1) is made. The matrix A does not appear in the local truncation error. However, lower error constants of the IMR scheme speak for the use of the IMR based scheme for most of the numerical examples that we have considered.

As mentioned above, the stability estimates alone are not enough to prove the high order accuracy of the deferred correction scheme. In order to rigorously determine the order of accuracy, the smoothness of the lower order accurate intermediate solutions needs to be further investigated. In the local truncation error, high order time derivatives are present. These are replaced by high order difference quotients of the lower order accurate solutions. The error made by replacing the derivatives of the exact solution by a difference quotient of the approximate solution needs to be of sufficiently high accuracy. As a consequence, stability estimates are required also for the difference quotients of the intermediate solutions. This is done both for the IMR and the BDF2 based scheme. The estimates are formulated for constant matrices A and a generalization to time-dependent A(t) is indicated. The main error estimate for the IMR based scheme is

**Theorem 2.** Let  $u^{2j,n}$  be the 2j-th order solution to the deferred correction method based on the implicit midpoint rule. Then the error  $e^{2j,n} = u(t_n) - u^{2j,n}$ 

satisfies

$$\begin{split} \|D_{+}^{p}e^{2j,n}\| &\leq const \Big( \max_{0 \leq i \leq j-1 \atop i \leq k \leq j-1} \|A^{3k+p-i}e^{2(j-k),0}\| \Delta t^{2k} \\ &+ \Delta t^{2j} \Big( \max_{0 \leq i \leq k \atop 1 \leq k \leq j} \|A^{l}u^{(2j+p+k-l)}(t)\| \\ &+ \max_{0 \leq s \leq N \atop 0 \leq i \leq j-1 \atop 0 \leq k \leq j-1 \atop 0 \leq l \leq 3k+p-i} \|A^{l}u^{(k+p-l+2j-i)}(s)\| \Big) \Big) + O(\Delta t^{2j+1}) \,. \end{split}$$

$$(3.2)$$

Here,  $t_v$  denotes a small number that depends on the deferred correction step j but not on  $t_n$  and the constant depends on  $t_n$  but not on A.

Here,  $u^{(k)}(t)$  denotes the k-th order time derivative of the solution to (3.1). The order of accuracy is 2j if the exact solution is sufficiently smooth and the operator  $A^l$  acting on the exact solution and its time derivatives results in a bounded vector, independent of  $\Delta x$ . Here, we need to consider  $l \leq 3(j-1)$ .

As mentioned before, if boundary conditions are incorporated in A, the action of A on a smooth vector will not give a bounded term. We present ways to reformulate the boundary conditions to guarantee boundedness of  $A^lu$  for sufficiently high powers l.

For the BDF2 based scheme, another aspect needs to be considered when investigating the smoothness of the intermediate solutions. The BDF2 scheme involves three time levels. In order to start the scheme, two initial conditions are needed. Usually, a one-step scheme is used to obtain the first time-step. For the deferred correction scheme, smoothness of the intermediate solutions is a crucial requirement. Using the above described startup procedure will usually render nonsmooth intermediate solutions. A method to obtain a second initial condition that guarantees sufficient smoothness in time is given. Another possible strategy might be a post processing to smoothen the intermediate solutions. In a series of numerical experiments, the results from the analysis are confirmed. The central issues studied in the experiments are the following:

- the choice of the second initial condition for the BDF2 based scheme,
- the formulation of the boundary conditions,
- behavior for time-dependent A(t) and
- performance for stiff problems.

The last point is important to justify the use of implicit methods. As implicit schemes are more expensive per time-step, they are only useful for problems, for which the CFL number for an explicit method is considerably more restrictive than the accuracy requirements. These problems are called stiff problems. We consider two kinds of stiff problems. The first kind is the class of problems where different timescales are present in the problem and only the slow scale is of interest. The CFL number is nevertheless dictated by the fast scale. A

simple example is the scalar ODE

$$u_t = -\lambda u + (-1 + \lambda)e^{-t} \quad \lambda \gg 1,$$
  
 $u(0) = 1.$  (3.3)

The problem has the solution  $u(t) = e^{-t}$ . The time-step restriction of an explicit scheme is usually of the form  $\lambda \Delta t \leq const$ . For large  $\lambda$ , this will require a very small time-step, whereas the solution is independent of  $\lambda$ . For satisfactory resolution, a moderately small time-step would here be sufficient. Another group of problems requiring implicit schemes is the class where geometrical constraints lead to very small spatial step sizes. The CFL condition will usually give a bound on the time-step in terms of the smallest space-step. This will again lead to unnecessary small time-steps. The deferred correction schemes work well for problems where geometrical constraints lead to small spacesteps. For problems like (3.3), the deferred correction scheme will not give good results. This is due to the fact that a fast scale will appear in the intermediate, lower order solutions, even though it is not present in the exact solution. The schemes are asymptotically of the correct order of accuracy. The error constants will, however, become very large. A possible way to remedy this might be the application of a filter to suppress the fast scale in the intermediate solutions.

#### 3.4 Time compact schemes

Another class of high order accurate time discretization methods that does not fall under the same category as the methods mentioned so far is the class of time compact schemes. It is different in that it does not use the method of lines approach. When formulating a lower order accurate finite difference discretization of a PDE

$$\frac{\partial u}{\partial t} = \mathcal{L}u,\tag{3.4}$$

where  $\mathcal{L}$  is a differential operator in space, one can calculate an expansion of the local truncation error in time and space. To obtain higher order methods, one can add discretized approximations of the lower order terms occurring in the local truncation error to the scheme. This works well for the spatial discretization. For the approximation of  $\frac{\partial u}{\partial t}$ , this approach will often result in unconditionally unstable schemes. To avoid this, another technique can be used. Instead of discretizing the time derivatives in the local truncation error directly, one can use the differential equation (3.4), to transfer time derivatives into spatial derivatives. One then discretizes the higher order spatial derivatives. This will lead to *time compact schemes*. They are both *one-step* and *one-stage* schemes.

This approach has been used by Numerov in [31] and [32] and by Tuomela in [39]. A similar approach has been used by Lax and Wendroff in [25]. A similar concept is the *modified equations approach*, see e.g. [5], [36] and [40]. The performance of the time compact scheme based on an explicit second order scheme applied to the wave equation has been studied in [13] and [17]. In the last part of this thesis, we consider a fourth order accurate time compact scheme based on an implicit unconditionally stable scheme.

#### 3.5 Paper VI

A problem that requires high order time stepping schemes is the long time integration of the wave equation. The standard formulation of the wave equation in one space dimension is

$$p_{tt} = a(x)(b(x)p_x)_x$$

for the pressure p. Instead of using the above equation, one can introduce the velocity u, with  $u_t = bp_x$  and obtain the following first order system for the pressure and the velocity. To generalize to the inhomogeneous equation, forcing functions F and G are added.

$$\begin{pmatrix} p \\ u \end{pmatrix}_{t} = \begin{pmatrix} 0 & a(x) \\ b(x) & 0 \end{pmatrix} \begin{pmatrix} p \\ u \end{pmatrix}_{x} + \begin{pmatrix} F \\ G \end{pmatrix}. \tag{3.5}$$

To obtain a high order accurate scheme in time and space, we first consider the implicit midpoint rule together with a second order centered difference scheme on a staggered mesh in space. To obtain a fourth order accurate scheme, the local truncation error is expanded in terms of the time and space-step,  $\Delta t$  and  $\Delta x$ . The lowest order terms are of order  $\Delta t^2$  and  $\Delta x^2$ . The time derivatives in the error are transformed using (3.5) resulting in terms that only include spatial derivatives and the forcing terms. A discretization of these terms is then added to the scheme resulting in a fourth order scheme in space and time. The width of the stencil in time is two time levels and the width in space is five grid points.

A stability analysis based on the energy method shows that the fourth order scheme is unconditionally stable. The stability estimate includes derivatives of the forcing functions.

Some numerical experiments are performed. First, the long term time integration is compared to the second order scheme. It is seen that the second order scheme behaves very poorly for some problems, whereas the error of the fourth order scheme stays very small in all cases. Fourth order accuracy is achieved.

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We then consider the two-dimensional wave equation. In a similar manner as for the one dimensional case, one can construct a time compact, fourth order accurate scheme. The scheme is tested on a problem with discontinuous coefficients a and b and nonsmooth initial data. We consider wave propagation in a domain with two different media with a nonsmooth initial function. Of course, a reduction of the order of accuracy is expected. As we do not have an exact solution to the problem, we can only compare the results to the solution on a very fine grid. Such a solution has been calculated by Gustafsson and Wahlund [16], based on the time compact explicit scheme discussed in [17]. It will be published in a forthcoming paper. A source of error in the solution to the discretized problem is the presence of small oscillations due to the nonsmoothness of the coefficients and initial data. Here, the discontinuous coefficients seem to lead to less problems — no visible oscillations are present than the nonsmoothness of the initial data, which leads to a visible oscillation around the discontinuity in the derivate. A local grid refinement is performed. It leads to smaller oscillations. Here, an advantage of an unconditionally stable scheme is seen. The very small space-steps in the refined area would require a significant decrease in the time-step, if an explicit scheme had been used.

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