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# Convergence Acceleration for Flow Problems

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# CONVERGENCE ACCELERATION FOR FLOW PROBLEMS

## SUMMARY

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**1. Introduction.** Numerical analysis is a relatively new discipline within the fields of science and engineering. Numerical methods have been used since the days of Euler and Lagrange in the 18th century, but it was the birth of digital computers in the 20th century that led to a breakthrough. Numerical methods usually require a large number of simple calculations, something at which computers are very good.

In this thesis, we are interested in the numerical solution of partial differential equations. Such equations arise in the modelling of many physical phenomena, for example propagation of sound-waves, heat-convection and the tunnelling of electrons. However, the usefulness of differential equations is not limited to the field of natural science, for example the raise and fall of stock-prices can be described using them.

Explicit solutions of partial differential equations are usually unobtainable. Numerical methods have made it possible to find highly accurate approximations in many important practical implications. For example, the aerodynamical aspects of a new aircraft or a car can be investigated before it is manufactured and the design of a new bridge can be tested before construction.

Also, a new branch of physics known as computational physics has emerged during the last few decades, serving as an important complement to theoretical and experimental physics. The same trend is evident in chemistry and biology. As a consequence, the need for efficient numerical methods is growing.

In this thesis, we focus on the numerical solution of equations governing fluid flows, such as the Euler and the Navier–Stokes equations. Computational fluid dynamics (CFD) is one of the oldest examples of computational physics. However, there are still a number of open questions. Existing techniques need to be understood and more efficient methods are required.

Our main concern is the efficient solution of system of equations that arise when partial differential equations are discretised. These systems are usually solved by iterative methods and we discuss different convergence acceleration techniques.

There is a trend in this thesis, and in the convergence acceleration community in general, to use an increased amount of information about the origin of the system of equations. Tailor-made convergence acceleration techniques often perform better than generic “black-box” techniques. Perhaps future convergence acceleration techniques be in-built into the discretisation method or even into the formulation of the differential equation itself. Paper D in this thesis is a step in that direction.

This summary is organised as follows. In Section 2, we discuss the physical laws of fluid flows. The solution strategy is discussed in Section 3, followed by a brief overview of some standard convergence acceleration techniques in Section 4. One of the main contributions in this thesis is the study of semicirculant preconditioners. This technique is presented in Section 5, while Sections 6, 7 and 8 summarise Paper A, B and C respectively. Our results show that semicirculant preconditioners may offer excellent performance for CFD applications.

In Section 9 we discuss preconditioning in the context of the theory of Green's functions, something that motivates the studies in Paper D and E. These papers are summarised in Sections 10 and 11, and we end with some conclusions in Section 12.

**2. Fluid Dynamics.** In this section we discuss the equations governing fluid flows. For a more detailed and complete discussion about CFD, we refer for example to [39].

The physical laws of fluid flows can be stated as a set of partial differential equations (PDE), known as the Navier–Stokes equations. The continuity equation

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho \mathbf{v}) = 0, \quad (2.1)$$

describes conservation of mass, the momentum equation

$$\frac{\partial(\varrho \mathbf{v})}{\partial t} + \nabla \cdot (\varrho \mathbf{v} \mathbf{v}) + \nabla p = \varrho \mathbf{F} + \nabla \cdot \boldsymbol{\sigma}, \quad (2.2)$$

states conservation of momentum, and according to the energy equation

$$\frac{\partial(\varrho E)}{\partial t} + \nabla \cdot (\varrho E + p) \mathbf{v} = \varrho \mathbf{F} \cdot \mathbf{v} + \nabla \cdot (\kappa \nabla T + \boldsymbol{\sigma} \cdot \mathbf{v}), \quad (2.3)$$

energy is conserved. Here,  $\mathbf{v}$  denotes the velocity vector,  $\varrho$  the density,  $p$  the pressure and  $E$  the total energy. The body force  $\mathbf{F}$ , the viscous stress tensor  $\boldsymbol{\sigma}$ , the temperature  $T$  and the thermal conductivity coefficient  $\kappa$  vary for different problem settings. We use  $D/Dt$  to denote the material derivative. A derivation of Navier–Stokes equations can be found in most textbooks on continuum mechanics, e.g. [32].

The system (2.1)-(2.3) is usually closed by an equation of state

$$p = (\gamma - 1) \varrho \left( E - \frac{1}{2} \mathbf{v} \cdot \mathbf{v} \right), \quad (2.4)$$

where  $\gamma$  is the ratio of specific heats.

There are several specific situations, which may allow for simplifications of equations (2.1)-(2.3). For instance, the density of a liquid normally remains almost unchanged for a wide range of pressures, and assuming constant density

leads to the incompressible Navier–Stokes equations. For flows where viscous effects are negligible, the Euler equations, derived by assuming inviscid flow, can be used.

The Reynolds number is a measure of viscosity, usually defined as

$$Re = \frac{U_\infty L \rho_\infty}{\mu_\infty}, \quad (2.5)$$

where  $L$  is the characteristic length, for instance the diameter of the channel for channel flow, and  $U_\infty$ ,  $\rho_\infty$ , and  $\mu_\infty$  are the free-stream values of the velocity, density, and first coefficient of viscosity respectively. For low Reynolds numbers, corresponding to highly viscous flows, the boundary layers in which velocity decreases from free-stream values to zero are thick. For higher Reynolds numbers the layers becomes thinner and the equations normally becomes harder to solve using a computational method.

The Reynolds number is also connected to the regularity of the flow. For low Reynolds number, the flow is usually laminar. Fluid particles move in smooth layers, sliding over particles in adjacent layers without mixing them. For high Reynolds number, the flow is more likely to be turbulent. Small disturbances then cause fluid particles to be intermingled in an irregular way.

The speed of sound  $c$  satisfies

$$c^2 = \gamma \frac{p}{\rho}. \quad (2.6)$$

In transition areas between supersonic flow, where  $|\mathbf{v}| > c$ , and subsonic flow, where  $|\mathbf{v}| < c$ , rapid changes of velocity, pressure and density, known as shocks, may occur. Such problems are often particularly hard to handle. Also, the case  $|\mathbf{v}| \ll c$ , that is, when sound-waves move much faster than the medium, demands a lot of the computational method. A possible simplification is to model this case by the incompressible Navier–Stokes equations, which do not allow for sound-waves at all.

Many physical systems have a steady state. For instance, the flow around an aircraft changes during take off and the initial phase of a flight, but after a while, when the plane has been cruising at constant speed and direction for some time, the flow around the aircraft does no longer vary in time. To find the steady state solution, it is sufficient to solve the time-independent Navier–Stokes or Euler equations.

In this thesis we are developing numerical methods for time-independent compressible subsonic flows. We consider viscous as well as inviscid problems. For viscous problems, governed by the Navier–Stokes equations, we are particularly interested in high Reynolds numbers, yielding thin boundary layers.

The work in this thesis is a step towards the treatment of realistic problem settings. Scalar model problems have earlier been thoroughly studied [21] [22] [23] [38] [17]. In Paper A, B and C we study linearised versions of the Navier–Stokes and Euler equations as well as the fully nonlinear Euler equations. The

linearised equations are similar to the nonlinear in many aspects. Also, one way of solving nonlinear problems is by the Newton method, where several linear problems have to be solved. Therefore, if the linearised problem cannot be solved in a fast and efficient way, there is little hope of solving the nonlinear one efficiently, and studying the linearised problem is a natural first step.

**3. Solution Strategy.** There are several discretisation methods available for partial differential equations, such as finite difference methods (FDM), finite element methods (FEM), finite volume methods (FVM), and pseudo-spectral methods, each one with its own pros and cons. It is not always easy to choose what method to use, and often the decisions are based on previous experience and availability of software. In the CFD community, finite difference and finite volume methods are often used, and there are many quite successful computer codes in which these methods have been implemented.

Discretising a time-independent system of partial differential equations, such as the linearised Navier–Stokes or Euler equations, yields a large system of equations

$$Bv = g. \tag{3.1}$$

Here,  $B$  is a discrete approximation of the partial differential operator, represented as a matrix. The boundary conditions have been included in  $B$  and in the discrete forcing function  $g$ . The solution  $v$  is a discrete approximation of the solution to the original problem.

Most of the execution time in a CFD code is spent on solving this system of equations. The goal in this thesis is to come up with a technique that not only speeds up such computations, but also can be added to existing computer codes without too much programming effort.

The finite difference and finite volume methods both yield a sparse matrix  $B$ , that is, a matrix with only a few non-zero elements per row. Furthermore, if the discretisation is made on a structured grid, the non-zero elements are gathered on a few diagonals, and only these diagonals have to be stored.

There are basically two different ways of solving a system of equations like (3.1). It can be done by a direct method, such as Gaussian elimination, or by using an iterative solver. However, for realistic application problems in several space dimensions, direct solvers often require too much memory and time.

The problem (3.1) can be solved iteratively by some non-stationary method from the linear algebra field, or by integrating the corresponding time-dependent problem

$$\frac{\partial v}{\partial t} + Bv = g, \tag{3.2}$$

in time until steady state has been reached. People working with CFD often choose the second approach. Both approaches result in methods where the most time-consuming operations are matrix-vector multiplications with  $B$ . Therefore,

the sparse representation discussed above can be used and the methods are memory lean.

In order to solve (3.2) we discretise in time, and advance the solution until it is sufficiently close to steady state. Since we are interested in the steady state solution only, the method does not have to be accurate in time. On the contrary, we would like to use large steps, so that steady state can be reached in as few iterations as possible.

There is a classical observation by Courant, Friedrichs and Lewy [11] regarding finite difference methods. They realised that a discretisation of a time-dependent PDE must allow information to be transported along characteristics. Otherwise, the discretisation does not approximate the PDE. If this condition is not met, the discrete solution will typically grow rapidly in time and “blow up”. The CFL-condition is therefore a stability condition. It relates the resolution in time to the resolution in space, and limits the time step for many discretisations.

Note that the CFL-condition is not a physical requirement, but rather a property of the discretisation method, related to how the method propagates information. Also, the CFL-condition is more limiting for problems where the solution changes rapidly in space. Because of accuracy reasons, a fine spatial grid must then be used, and the CFL-condition implies that a small step must be used also in time.

To conclude, the CFL-condition forces us to use a small step in time and do a lot of iterations, even though we are not interested in how the solution evolves before it reaches steady state.

A large number of sophisticated iterative methods have been developed during the years in order to overcome this problem. Our approach is to continue to use a very simple iteration, but combine it with preconditioning. Instead of solving (3.2), we solve

$$\frac{\partial v}{\partial t} + M^{-1}Bv = M^{-1}g, \quad (3.3)$$

for some preconditioning matrix  $M^{-1}$ . The steady-state solution is the same, but the convergence rate depends on  $M^{-1}B$  instead of  $B$ . A good preconditioner can improve convergence considerably, without adding too much work and storage.

In Paper A, B and C we examine a preconditioner based on semicirculant approximations. We construct a matrix  $M$  that approximates  $B$  and has the property that the inverse  $M^{-1}$  can be applied using the fast Fourier transform (FFT). Our analysis of model problems shows that the composition  $M^{-1}B$  is close to the identity matrix in the sense that an iterative method converges in a small number of iterations.

In Paper D, our approach is slightly different. Here, we construct an integral operator  $K$  that approximates the inverse of the differential operator, and use a discretisation of  $K$  as preconditioner.

In both cases, the idea is to change the properties of the problem by a transformation instead of improving the iterative method. Both experiments

and analysis show that a very basic iteration scheme, such as the forward Euler method can be used.

**4. Convergence Acceleration.** In this section we give a brief overview of some convergence acceleration techniques. The term “convergence acceleration” is sometimes used in other contexts, such as the derivation of high order numerical integrators by Richardson extrapolation techniques. Here, we use the term to denote the art of improving convergence of iterative solvers.

We also use “preconditioning” as a synonym to convergence acceleration. This term was used by Turing in 1948 [41], but the first application of the word to the idea of improving convergence of an iterative method is probably by Evans in 1968 [14].

Iterative methods based on matrix splitting, such as the Jacobi and the Gauss-Seidel methods can be viewed as preconditioned fixed point iterations. In this sense, convergence acceleration techniques have been used for almost two hundred years.

It is interesting to note that the development of iterative methods has walked hand in hand with the development of preconditioners. When the conjugate gradient (CG) algorithm was proposed by Hestenes and Stiefel in 1952, the idea of preconditioning also appeared implicitly [19]. However, it was not until later, after publications such as [10] and [35], that the preconditioned CG method became widely used. Other early applications are described in [31]. Today, much as a result of the development of efficient preconditioning techniques, the CG algorithm has become a widespread and popular iterative method. For a complete history of the CG algorithm, see [15].

The construction of preconditioners by using incomplete factorisations was first suggested by Varga [44], but has been discussed by a number of people. The idea became popular when it was used by Meijerink and van der Vorst [35] to generate preconditioners for the CG algorithm. A number of factorisations, such as the incomplete Cholesky factorisation, the incomplete LU factorisation and the incomplete QR factorisation has been tried and proved to be successful in a range of applications. Sparse approximate inverses have also been proposed as preconditioners, see for instance [1] [2] [3] [34]. This kind of preconditioners are better suited for parallel computers.

Preconditioners based on matrix splittings, incomplete factorisations and sparse approximate inverses are designed for general classes of matrices, such as symmetric positive definite matrices or  $M$ -matrices. Alternatively, preconditioners can be designed for broad classes of underlying problems, such as differential equations or integral equations. Examples of problem specific preconditioners that has been applied to CFD problems are preconditioning of the system of PDE [42], local time stepping [27], implicit residual smoothing [13] [26], and multigrid [26]. Both multigrid and domain decomposition preconditioners [9] were initially used for elliptic partial differential equations, but has successfully been applied to other kinds of PDE.

In Paper D we introduce a class of preconditioners based on theory of partial differential equations. A similar train of thought can be found in [29] and [33], where Kay, Loghin and Wathen use knowledge about the Green's function for preconditioning the convection-diffusion equation and the Navier–Stokes equations. Here, information about the differential equation is used when constructing an approximate inverse of the matrix, or a part of the matrix, while we on the other hand approximate the inverse of the differential operator. Both approaches are examples of problem specific preconditioners.

There is a very fine line between the two different approaches. For example, the algebraic multigrid method [5] generalises the multigrid method to systems of equations that not necessarily are discretisations of differential equations. Also, techniques have been developed for matrices with certain structures, such as constraint preconditioning [30] and semicirculant preconditioning. Semicirculant preconditioners is one of the main topics of this thesis, and we devote the next section to a presentation of this technique.

**5. Semicirculant Approximations.** The technique of semicirculant preconditioning has its origin in the use of circulant preconditioners for Toeplitz systems of equations, which was proposed in the late 80s [40] [8] [43]. A review of this area is available in [7]. The semicirculant technique has been developed for hyperbolic and almost hyperbolic PDE problems [21] [22] [23] [24] [25] [17], as well as elliptic problems [6]. Much work has been spent on implementation aspects [20] [28] [36]. Theory has also been developed [22] [23] [38], where favourable convergence properties for the preconditioned system of equations are proved.

Finite difference and finite volume approximations are local approximations, that is, the derivative at a certain point is estimated by values at neighbouring points. This is the reason why  $B$  is structured in the way described in Section 3. Furthermore, if the grid points are numbered lexicographically,  $B$  also has a certain block structure. An example for the two-dimensional isentropic Euler equations is shown in Figure 5.1. There are three block levels, corresponding to the two space dimensions and the system of PDE. The size of the inner blocks is given by the number of unknown functions in the PDE. In this example we solve for the Cartesian velocity components  $v_1$  and  $v_2$  and the density  $\rho$ . Hence, the inner blocks are  $3 \times 3$ . The structure of the outer levels depend on the number of grid points and the discretisation method.

A semicirculant approximation of  $B$  is constructed by modifying the structure at the middle level, making it periodic, see Figure 5.2. Furthermore, the entries in the blocks have been replaced by some constant values along the diagonals. The matrix blocks then have a circulant structure. A matrix that is circulant at some, but not all levels is said to be semicirculant. The constant diagonal values are chosen so that the Frobenius norm

$$\|M - B\|_F$$

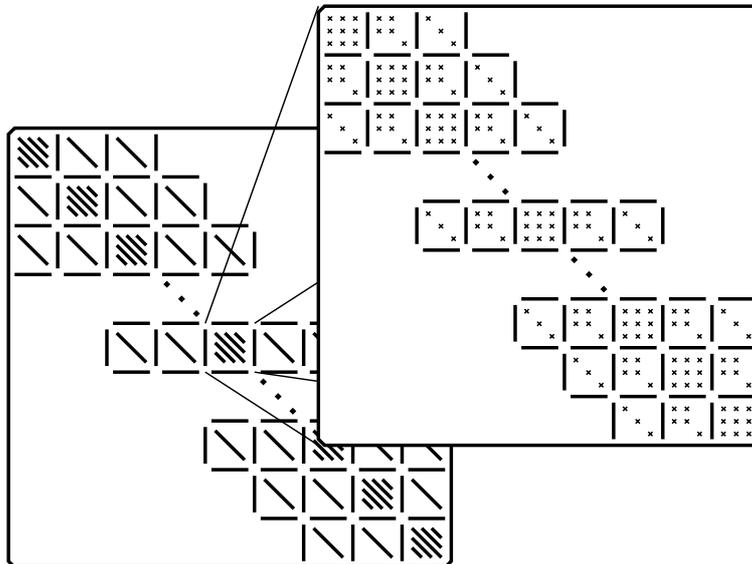


FIG. 5.1. *The structure of the coefficient matrix  $B$  for the 2D linearised Euler equations discretised using centred finite differences.*

is minimised, something that can be done with little computational effort [24]. In fact, the only calculation required is that of computing mean values of diagonals in  $B$ .

The matrix  $M$  represents, by construction, an operator with constant coefficients and periodic boundary conditions in one direction. Because of this, the inverse can be applied, that is, the equation  $My = x$  can be solved, in the following three steps. First, a number of independent FFTs are computed in the direction with periodic boundary conditions. The transformed problem consists of a number of independent systems of equations, which are solved in the second step. The transformed solution is then transformed back via a number of independent inverse fast Fourier transformations in the third and final step.

Since  $M^{-1}$  can be applied using FFTs, the preconditioner solve is relatively cheap. For the linearised Euler and Navier–Stokes equations, the time needed for applying the preconditioner is comparable to that of a few residual evaluations. Note that the algorithm is very well suited for parallel implementation, since in each step of the algorithm a number of operations can be done independent of each other [20].

The preconditioning matrix  $M$  can be viewed as an approximation of a partial differential operator with periodic boundary conditions and constant coefficients in one dimension. How well  $M$  approximates  $B$  can be related to the difference between the solution of the original and modified problems. Let  $v$  be

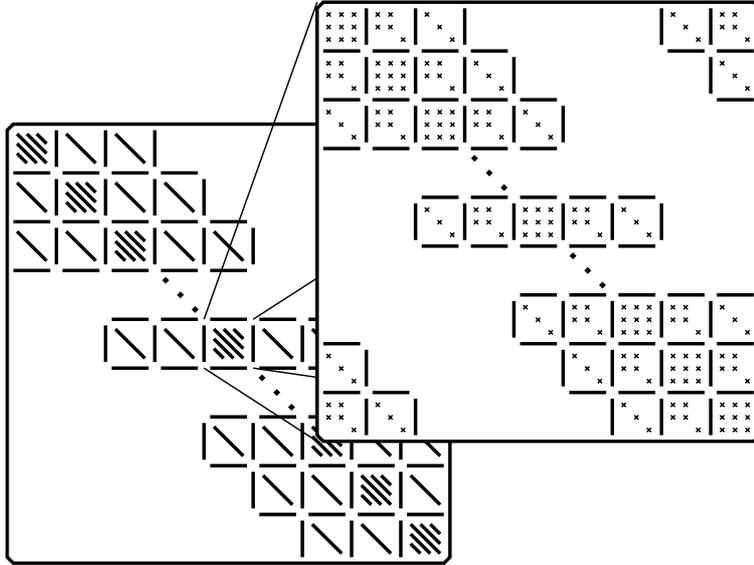


FIG. 5.2. The structure of the semicirculant approximation  $M$  of the matrix  $B$  shown in Figure 5.1.

the solution of

$$Bv = g,$$

and let  $\tilde{v}$  be the solution of

$$M\tilde{v} = g.$$

Since

$$\|\tilde{v} - v\| = \|M^{-1}g - v\| = \|M^{-1}Bv - v\| \leq \|M^{-1}B - I\| \|v\|,$$

or equivalently

$$\frac{\|\tilde{v} - v\|}{\|v\|} \leq \|M^{-1}B - I\|,$$

we see that the relative difference between the solutions yields a lower bound on how well the inverse of  $M$  may approximate the inverse of  $B$ .

By this argument, we realise that if the periodic-constant coefficient approximation is used in a direction where the solution is far from periodic,  $M^{-1}B$  will not be a close approximation of the identity matrix. It is still possible that  $M^{-1}$  serves as a good preconditioner. In fact, some convergence acceleration techniques, such as constraint preconditioning [30], do not try to approximate

the inverse and still shows excellent performance. However, a reasonable goal is to approximate the inverse as well as possible.

Consider viscous flow over some body, such as an aircraft. For high Reynolds numbers, the velocity varies from free-stream value to zero in a thin boundary layer. We then employ the approximations in the direction parallel to the surface, but not in the normal direction.

It is possible to use a preconditioner which employs the periodic–constant approximation in both directions. However, for many applications, such as boundary layer flows, the operator cannot be well approximated in one direction, and since the cost of keeping one dimension unaltered is negligible, we prefer this approach.

The extension to three dimensions is straightforward. For a three-dimensional problem, there will be another block level outside the two levels shown in Figure 5.1. The preconditioner  $M$  may then be constructed so that it becomes circulant on two of the levels.

**6. Paper A.** In Paper A, we examine the linearised and symmetrised Euler equations

$$A_1 \frac{\partial \mathbf{u}}{\partial x_1} + A_2 \frac{\partial \mathbf{u}}{\partial x_2} + A_3 \mathbf{u} + \mathbf{F} = 0, \quad (6.1)$$

where  $\mathbf{u} = (\varrho, v_1, v_2)^T$  is the departure from an approximation  $\mathbf{U} = (R, V_1, V_2)^T$ ,

$$A_1 = \begin{pmatrix} V_1 & c & 0 \\ c & V_1 & 0 \\ 0 & 0 & V_1 \end{pmatrix}, \quad A_2 = \begin{pmatrix} V_2 & 0 & c \\ 0 & V_2 & 0 \\ c & 0 & V_2 \end{pmatrix},$$

$$A_3 = \begin{pmatrix} \frac{\partial V_1}{\partial x_1} + \frac{\partial V_2}{\partial x_2} & \frac{c}{R} \frac{\partial R}{\partial x_1} & \frac{c}{R} \frac{\partial R}{\partial x_2} \\ \frac{V_1}{V_1} \frac{\partial V_1}{\partial x_1} + \frac{V_2}{V_2} \frac{\partial V_1}{\partial x_2} & \frac{\partial x_1}{\partial V_1} & \frac{\partial x_2}{\partial V_1} \\ \frac{c}{V_1} \frac{\partial x_1}{\partial V_2} + \frac{c}{V_2} \frac{\partial x_2}{\partial V_2} & \frac{\partial x_1}{\partial V_2} & \frac{\partial x_2}{\partial V_2} \\ \frac{c}{c} \frac{\partial x_1}{\partial x_1} + \frac{c}{c} \frac{\partial x_2}{\partial x_2} & \frac{\partial x_1}{\partial x_1} & \frac{\partial x_2}{\partial x_2} \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} c \frac{\partial V_1}{\partial x_1} + c \frac{\partial V_2}{\partial x_2} \\ V_1 \frac{\partial V_1}{\partial x_1} + V_2 \frac{\partial V_1}{\partial x_2} \\ V_1 \frac{\partial V_2}{\partial x_1} + V_2 \frac{\partial V_2}{\partial x_2} \end{pmatrix}.$$

Here,  $v_1$  and  $v_2$  denote the Cartesian velocity components. The pressure has been eliminated using relation (2.6), where  $\gamma = 1$  has been employed.

We consider flow in a narrowing channel, and compute the approximate solution  $\mathbf{U}$  by solving a potential flow problem. For low Mach numbers, that is when  $|\mathbf{v}| < c$ ,  $\mathbf{U}$  is a good approximation of the solution to (6.1).

Equation (6.1) is discretised on an orthogonal grid using second order finite difference approximations, where fourth order artificial viscosity is added.

We compare the semicirculant preconditioning technique to a standard multigrid iteration. A grid refinement study shows that both the forward Euler method combined with a semicirculant preconditioner and the multigrid method

converge in a number of iterations which is bounded as the number of grid points is increased. However, the number of arithmetic operations required is shown to be less for the preconditioned forward Euler method.

We also examine the time-independent Kreiss equation

$$\frac{\partial u}{\partial x_1} + \frac{\partial u}{\partial x_2} = 0, \quad (6.2)$$

solved on the unit square, where  $u(x_1, 0)$  and  $u(0, x_2)$  are prescribed. This problem serves as a model problem for the Euler equations. An analysis shows that the spectrum of the preconditioned operator is bounded, also as the number of grid points approaches infinity. We show that the forward Euler method can be used with a constant time-step, independent of the number of grid points.

We also show that under certain conditions, it is possible to use an arbitrarily small artificial viscosity. Numerical experiments show that the same is true for the linearised Euler equations. The semicirculant preconditioner is robust in the sense that the amount of artificial viscosity can be varied, which is not true for the multigrid method.

**7. Paper B.** In Paper B, we consider the linearised Navier–Stokes equations,

$$A_1 \frac{\partial \mathbf{u}}{\partial x_1} + A_2 \frac{\partial \mathbf{u}}{\partial x_2} = B_1 \frac{\partial^2 \mathbf{u}}{\partial x_1^2} + B_2 \frac{\partial^2 \mathbf{u}}{\partial x_2^2} + B_3 \frac{\partial^2 \mathbf{u}}{\partial x_1 \partial x_2} + \mathbf{F}, \quad (7.1)$$

where

$$A_1 = \begin{pmatrix} V_1 & 0 & \frac{\kappa}{R} \\ 0 & V_1 & 0 \\ R & 0 & V_1 \end{pmatrix}, \quad A_2 = \begin{pmatrix} V_2 & 0 & 0 \\ 0 & V_2 & \frac{\kappa}{R} \\ 0 & R & V_2 \end{pmatrix},$$

$$B_1 = \mu \begin{pmatrix} \frac{4}{3} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad B_2 = \mu \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{4}{3} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad B_3 = \mu \begin{pmatrix} 0 & \frac{1}{3} & 0 \\ \frac{1}{3} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Here, the solution  $\mathbf{u} = (v_1, v_2, \rho)^T$  is the departure from the approximate solution  $\mathbf{U} = (V_1, V_2, R)^T$ , around which (7.1) has been linearised. The function  $\mathbf{F}$  is a sum of partial derivatives of  $V_1$  and  $V_2$ . The pressure has been eliminated in the same way as for the linearised Euler equations.

We are interested in the performance of the semicirculant preconditioning technique for boundary layer problems, and we solve (7.1) for flow over flat plate, a well known model problem in fluid dynamics. The solution is well approximated by the so called Blasius-solution, which is the solution of the incompressible problem. We use this solution to determine  $V_1$  and  $V_2$ .

Problem (7.1) is discretised using a finite volume method on a stretched grid, which is designed to resolve the boundary layer close to the plate. We perform three different numerical experiments, where we compare the semicirculant preconditioner to a standard multigrid method.

The first experiment is a grid refinement study, where the Reynolds number is fixed. This setting is well suited for the multigrid method, but still, the forward Euler method combined with semicirculant preconditioning turns out to require less computational work as long as the problem size is not too large.

In the second experiment, we vary the Reynolds number, and refine the grid only to ensure a certain accuracy requirement in the boundary layer. In this case the semicirculant preconditioner is a clear winner. The time step for the forward Euler method can be chosen as a constant, independent of the Reynolds number. If however, the grid is stretched not only in the direction perpendicular to the plate, but also parallel to the plate, the performance of the semicirculant preconditioner becomes less favourable. When the stretching is very large, we conclude that this technique should not be used.

The third experiment is designed to illustrate the robustness of the semicirculant preconditioning technique. By varying the amount of artificial viscosity we find that the number of iterations needed for convergence is changed only slightly. The multigrid technique, on the other hand, does not converge if the amount of artificial viscosity is decreased.

We also analyse a relevant model problem, namely the following advection-diffusion equation

$$\begin{aligned} \frac{\partial u}{\partial x_1} + \sqrt{\epsilon} \frac{\partial u}{\partial x_2} &= \epsilon \frac{\partial^2 u}{\partial x_2^2}, & 0 < x_1, x_2 < 1 \\ u(x_1, 0) &= 1, & 0 < x_1 < 1 \\ u(x_1, 1) &= 0, & 0 < x_1 < 1 \\ u(0, x_2) &= 1 - x_2^2, & 0 < x_2 < 1. \end{aligned} \tag{7.2}$$

The PDE (7.2) is discretised on a uniform grid, using centred finite difference approximations. We show that under certain conditions the asymptotic spectrum is bounded. Furthermore, the forward Euler method can be applied to the preconditioned problem using a constant time step, independent of the space step as well as the physical viscosity parameter  $\epsilon$ .

**8. Paper C.** In paper C, we consider the non-linear Euler equations

$$A_1(\mathbf{u}) \frac{\partial \mathbf{u}}{\partial \mathbf{x}_1} + A_2(\mathbf{u}) \frac{\partial \mathbf{u}}{\partial \mathbf{x}_2} = 0, \tag{8.1}$$

where  $\mathbf{u} = (\varrho, v_1, v_2)^T$ ,  $\varrho$  is the density and  $v_1$  and  $v_2$  are the velocity components. Furthermore,

$$A_1(\mathbf{u}) = \begin{pmatrix} v_1 & \varrho & 0 \\ c^2/\varrho & v_1 & 0 \\ 0 & 0 & v_1 \end{pmatrix}$$

and

$$A_2(\mathbf{u}) = \begin{pmatrix} v_2 & 0 & \rho \\ 0 & v_2 & 0 \\ c^2/\rho & 0 & v_2 \end{pmatrix},$$

where  $c$  is the speed of sound. Once again, the pressure has been eliminated by the use of relation (2.6).

We consider subsonic flow in a narrowing channel and discretise Equation (8.1) using second order centred finite differences and a fourth order artificial viscosity.

The system of equations is preconditioned by the semicirculant approximation technique and integrated in time with the forward Euler method until steady state has been reached. The experiments show that the favourable convergence properties of the semicirculant convergence acceleration technique are retained. The time step is not limited by a CFL-criterion. On the contrary, the time step can be chosen independent of the space step, and the iterations converge in a fixed number of steps.

Implementation issues are discussed and it is shown that the technique can be combined with a variety of iterative solvers. In particular, we consider non-linear Runge-Kutta methods, Picard iterations and the augmented Newton method. The convergence acceleration technique is shown to be robust with respect to the amount of artificial viscosity. Also, the preconditioner can be constructed as an approximation of a difference operator with second order viscosity

**9. Preconditioning Techniques and Green's Functions.** The semicirculant preconditioning technique has its origin in the field of numerical linear algebra, and it is very natural to present the idea by using matrices and other tools within the field. In fact, this view has proven itself to be useful both from an implementational and a theoretical point of view. However, it is not the only way of describing semicirculant preconditioners. In this section we will discuss semicirculant approximations in the context of Green's function theory. The presentation is intended to build a bridge between the discrete problem and the original differential equation. We will relate the semicirculant preconditioner, which is constructed from the discretised equation, to the kind of preconditioners studied in Paper D, that are constructed before discretisation, studying the differential operator itself.

Consider a system of  $n_c$  partial differential equations

$$Pu = f, \quad x \in \Omega \subset \mathbb{R}^d,$$

together with some boundary conditions on the boundary of  $\Omega$ . The differential equation has to be satisfied only inside the domain, and we assume  $\Omega$  to be open.

A Green's function  $G(x, y)$  is a matrix that, as a function of  $x$ , satisfies

$$PG(x, y) = I\delta(x - y), \quad x, y \in \Omega,$$

together with homogeneous boundary conditions. Here,  $I$  is the identity matrix of size  $n_c \times n_c$ , and  $\delta$  is the Dirac measure.

From the superposition principle, it follows that the integral operator  $K$ ,

$$Ku(x) = \int_{y \in \Omega} G(x, y)u(y) dx, \quad x \in \Omega,$$

is a right inverse of  $P$  on the space of functions satisfying homogeneous boundary conditions. On the same space,  $K$  is also a left inverse of  $P$ . This follows from  $G(y, x)$  being a Green's function to the adjoint problem. For details, we refer to Appendix A in Paper E.

The theory for systems of difference equations is similar. The differential operator is replaced by a difference operator  $P_h$ , the Dirac measure is replaced by the discrete delta function, and the integral in the definition of  $K$  is replaced by a sum. However, the essence of the theory is still the same; The inverse can be represented by a Green's function.

When a semicirculant preconditioner is used, the inverse of a modified difference operator  $\tilde{P}_h$  is applied. Original boundary conditions are replaced by periodic boundary conditions in one or several dimensions, and the coefficients are constant in these dimensions.

In Paper D, the approximation is not performed on the discrete level. Instead, we approximate the differential operator  $P$  by some operator  $\tilde{P}$  that can be easily inverted. A discretised version of the inverse is then used as a preconditioner. Here, we choose  $\tilde{P}$  as a constant coefficient operator and neglect the influence of boundary conditions. It is then possible to find a Green's function that satisfies

$$G(x, y) = E(x - y),$$

for some matrix  $E$ . Here,  $E$  is usually referred to as a fundamental solution. There are two main advantages of using fundamental solutions. First, they are explicitly known for many differential operators, and we do not have to compute the inverse of  $\tilde{P}$ . Secondly,  $K$  is a convolution operator, and a discrete version of the operator can be applied in an inexpensive way using FFT, at least on equidistant grids.

Before giving a more detailed description of this preconditioner we note that  $\tilde{P}$  could obviously also be constructed by replacing coefficients in one or more dimensions by constant coefficients and substituting the boundary conditions by periodic boundary conditions in these dimensions, that is, by using exactly the same procedure as when constructing a semicirculant approximation.

The two approaches, that is, performing the semicirculant approximation before and after discretisation, are obviously related. One interesting question is to what extent the approaches are the same. Will the Green's function  $\tilde{G}_h$  of the modified difference operator  $\tilde{P}_h$  approach the Green's function  $\tilde{G}$  of the modified differential operator  $\tilde{P}$  when the grid is refined? Such a convergence result

would be convenient since then it would be possible to analyse semicirculant preconditioners in an alternative way. Instead of considering  $P_h$ ,  $\tilde{P}_h$  and  $G_h$ , we could look at  $P$ ,  $\tilde{P}$  and  $\tilde{G}$ , and it would give an understanding about the way semicirculant preconditioners behave, at least for sufficiently large grids.

Considering the importance of Green's functions in the theory of partial differential equations, they may presumably play an equally important role when understanding numerical methods such as finite difference and finite volume discretisations. In particular, Green's functions theory can most likely shed some light on many stability and convergence issues. Studies concerned with the convergence of Green's functions have been performed, see e.g. [4] [16] [37], but the number of investigations is surprisingly small.

A necessary requirement for convergence of the discrete Green's function to the Green's function of the differential equation is that boundary conditions are chosen in such a way that the discretisation is stable. Thus, with properly chosen boundary conditions, there is a good chance that  $G_h$  converges to  $G$ . However, we are more interested in the convergence of the Green's function to the modified finite difference equation. This problem has another set of boundary conditions, which were designed to make the operator invertible with the fast Fourier transform technique, and no stability considerations were made. Therefore, there is little hope that the modified problem is stable, and  $\tilde{G}_h$  will only rarely converge to  $\tilde{G}$ . In fact, periodic boundary conditions may yield a problem that is not even well posed and  $\tilde{G}$  may fail to exist, while  $\tilde{G}_h$  is perfectly well defined.

To summarise, the alternative analysis suggested above is not possible because of stability issues. The modified finite difference equation is not stable, and the Green's function will be contaminated with parasitic solutions that fail to vanish as the grid is refined.

However, there is still hope for an asymptotic analysis based on theory of differential rather than difference operators. Already in 1959, Dahlquist showed that the parasitic parts of the discretisation error for linear multi-step methods have smooth components that asymptotically satisfy modified differential equations [12]. The result can also be found in Henrici's book [18], see for example Theorem 5.12. In paper E, we generalise this observation to boundary value problems.

In the future, we hope to be able to generalise the idea also to partial differential equations, and with this type of tools, it would be possible to represent both the true and the parasitic parts of  $\tilde{G}_h$  by functions satisfying certain differential equations. The study in Paper D, where the main part of the analysis is derived for differential and integral operators instead of the corresponding discrete operators, shows that this kind of analysis is powerful. It gives an insight and understanding of the preconditioning technique that is difficult to achieve by considering the discrete problem. Thus, an asymptotic analysis of semicirculant preconditioners will probably increase our understanding of the technique.

**10. Paper D.** In paper D, we consider a scalar PDE

$$Pu = f, \quad x \in \Omega, \quad (10.1)$$

where  $P$  is a linear operator with constant coefficients, and  $\Omega$  is an open, bounded domain in  $\mathbb{R}^d$ .

We assume  $q$  boundary conditions to be given on the form

$$B_k u = g_k, \quad x \in \Gamma_k \subset \partial\Omega, \quad k = 1, \dots, q, \quad (10.2)$$

where  $B_k$  are linear partial differential operators with constant coefficients.

By scaling the boundary conditions, both the PDE (10.1) and the boundary conditions (10.2) can be written as a single equation

$$Pu + Bu = f + g, \quad x \in \mathbb{R}^d, \quad (10.3)$$

where

$$B = \sum_{k=1}^q \delta_{\Gamma_k} B_k \quad \text{and} \quad g = \sum_{k=1}^q \delta_{\Gamma_k} g_k.$$

Here,  $\delta_{\Gamma_k}$  denote the Dirac measure with support on  $\Gamma_k$ . The reformulation is an attempt to find a form well suited for preconditioning with integral operators.

We choose  $K$ ,

$$Ku(x) = \int_{y \in \Omega} E(x-y)u(y)dx, \quad x \in \Omega,$$

where  $E$  is a fundamental solution of  $P$ , as a preconditioner. By this choice,  $K$  is the inverse of  $P$  when  $\Omega = \mathbb{R}^d$ . Hopefully,  $K$  is a good approximation of the inverse when  $\Omega$  is a true subset of  $\mathbb{R}^d$ , and boundary conditions are given. The operator  $K$  is also a convolution operator, and we give an algorithm for applying a discretised version of the operator in a non-expensive way by the use of FFT.

Our analysis shows that for first order PDE with boundary conditions not involving any derivatives, the preconditioner is successful in the sense that the preconditioned operator  $K(P+B)$  is bounded. Unfortunately, for equations of higher order than one, this result no longer holds.

We perform numerical experiments on both the convection equation, which is first order, and the convection-diffusion equation, which contains second order derivatives. The preconditioned problem is solved by a fixed point iteration equivalent to the forward Euler method with  $\Delta t = 1$ .

For the convection equation, the fundamental solution is singular along a line, causing some problems in the discretisation of  $K$ . It turns out that the best results are achieved when using some artificial diffusion and a preconditioner based on the fundamental solution of the advection-diffusion equation. We then

get convergence in a fixed number of iterations, independent of the number of grid points.

As predicted by the theory, the norm of the preconditioned operator for the second order convection-diffusion equation grows as the mesh is refined, and the number of iterations required for convergence increases accordingly. However, if the grid is chosen to give a fixed number of grid points within boundary layers, the number of iterations is independent of the physical viscosity parameter. Interestingly enough, the same result was achieved using a semicirculant preconditioner in paper B.

**11. Paper E.** In paper E, we consider a finite difference approximation

$$\begin{aligned} P_h v &= f_h, \\ B_{k,h} v &= g_{k,h}, \quad k = 1, \dots, p+q, \end{aligned} \quad (11.1)$$

of a linear two point boundary value problem

$$\begin{aligned} Pu &= f, \\ B_k u &= g_k, \quad k = 1, \dots, p, \end{aligned} \quad (11.2)$$

where  $P$  is a differential operator of order  $p$  and  $P_h$  is a finite difference operator with stencil width  $p+q+1$ . Equation (11.2) requires  $p$  boundary conditions, and (11.1) requires an additional  $q$  numerical boundary conditions.

We show that the finite difference equation (11.1) is closely related to a certain system of differential equations

$$\begin{aligned} Pu^{(0)} &= f, \\ P_{z_j} u^{(j)} &= 0, \quad j = 1, \dots, q, \\ B'_k u &= g'_k, \quad k = 1, \dots, p+q. \end{aligned} \quad (11.3)$$

From theory of ordinary differential equations, we know that the solutions of (11.3) depend continuously on  $f$  and  $g'_k$ . We show that  $v$  also depends continuously on  $f$  and  $g'_k$ . Using this property, we prove that  $v$  approaches the function

$$u^{(0)}(x_i) + \sum_{j=1}^{q_l} z_j^i h^{p-1} u^{(j)}(x_i) + \sum_{j=q_l+1}^q z_j^{i-N} h^{p-1} u^{(j)}(x_i), \quad (11.4)$$

when  $h$  tends to zero. Here,  $u^{(0)}, \dots, u^{(q)}$  satisfy (11.3), and  $z_j$  are characteristic roots of the principal part of the finite difference operator  $P_h$ . The roots  $z_j$  have been ordered in such a way that  $|z_j| \leq 1$ ,  $z_j \neq 1$ , for  $j = 1, \dots, q_l$ , and  $|z_j| > 1$  for  $j = q_l + 1, \dots, q$ . Characteristic roots equal to one are not included. The first term in (11.4) is the true solution and the other terms are parasitic.

There are three possible reasons why the discrete solution may fail to converge.

1. The finite difference equation (11.1) may not have a unique solution. In this case, there is no unique solution of (11.3).

2. The boundary data  $g'_k$  of system (11.3) may not exist. These numbers are the limits as  $h$  tends to zero of boundary data  $g_{k,h}$ , scaled in a certain way. In this case, (11.3) is not even well defined.
3. If (11.3) has a unique solution, it may still happen that at least one of the functions  $u^{(j)}(x)$ ,  $j = 1, \dots, q$ , is different from zero. Then, if  $p = 1$ , the parasitic part will not vanish when  $h$  tends to zero.

In all three cases it is sufficient to study the system (11.3).

In this context, it is easy to construct boundary conditions that give a convergent solution. One could for instance use a consistent approximation of

$$\begin{aligned} B_k u^{(0)} &= g_k, & k &= 1, \dots, p, \\ u^{(j)}(0) &= 0, & j &= 1, \dots, q_l, \\ u^{(j)}(1) &= 0, & j &= q_l + 1, \dots, q. \end{aligned} \tag{11.5}$$

We derive estimates of the accuracy showing that full approximation order is necessary only for the true boundary conditions.

The choice of boundary conditions is in no way unique. There are many sets that give solutions converging with expected order of accuracy. However, note that the main goal of this paper is not to construct numerical boundary conditions but to achieve a better understanding of the finite difference method. This understanding may be used in many different applications, and the study of numerical boundary conditions illustrate the power of the new theory.

**12. Conclusions.** In this thesis we consider the numerical solution of CFD problems. We are interested in time-independent compressible subsonic flow, and we study both viscous and inviscid problems, represented by the Navier–Stokes and the Euler equations respectively. In this work we study linearised as well as non-linear problems.

The partial differential equations are discretised using a finite difference or finite volume method on a structured grid, which is a common approach in the CFD community. In the linear case, the result is a large system of equations

$$Bv = g,$$

where the coefficient matrix  $B$  is sparse and structured. Our goal is to construct a preconditioning technique that can be easily implemented in existing codes, and in Paper A, B and C we construct such a preconditioner by using semicirculant approximations of  $B$ . The inverse of such an approximation  $M$  can be applied using fast Fourier transforms. In this thesis we show that the preconditioned problem

$$M^{-1}Bv = M^{-1}g$$

can be solved with some simple iteration, such as the forward Euler method, in an efficient way.

The results for the Euler and the Navier–Stokes equations are similar. For both problems we find that the forward Euler method, applied to the preconditioned problem, is not limited by a CFL-condition. A time step, independent of the number of grid points can be used for the Euler equations. The same is true for a wide range of grid sizes for the Navier–Stokes equations. Here, the time step is also independent of the Reynolds number.

The semicirculant preconditioning technique is compared to a standard multigrid iteration. Multigrid also shows grid independent convergence, but requires a larger number of arithmetic operations. Also, there are a number of parameters, such as the number of grid levels, the CFL-number and the amount of artificial viscosity, which must be carefully chosen to ensure good performance. The preconditioned forward Euler method operates on one grid only, the time step can be chosen as a constant and the technique is robust in the sense that the amount of artificial viscosity may be varied.

In Paper D we use a slightly different approach. Here, the preconditioner is based on an approximation of the partial differential equation, rather than the discrete finite difference equation. By this approach, we use a lot of information about the origin of the problem when constructing the preconditioner, and it becomes-tailor made for the particular problem. Also, we separate the construction and analysis into two different steps. First, we try to find an integral operator that is a good approximation of the differential operator, and then, in the second step, we consider complications due to discrete phenomena.

Both theory and experiments proves that the preconditioner can be used for first order scalar PDE such as the convection equation. It turns out that a simple fixed point iteration can be used and convergence is achieved in a fixed number of iterations, independent of the number of grid points.

The last paper, Paper E, should be viewed as the first step towards an asymptotic analysis of the finite difference method. In particular, we are interested in building a bridge between the discrete and the continuous problem. In Paper D, the main part of the analysis of the preconditioning technique is derived for differential and integral operators instead of the corresponding discrete operators. The study shows that this kind of analysis is powerful and gives an insight and understanding of the preconditioning technique that is hard to achieve by considering the discrete problem. Thus, an asymptotic analysis of semicirculant preconditioners will probably increase our understanding of the technique.

In paper E we consider two point boundary value problems, and prove that the parasitic solutions have smooth components that asymptotically satisfies modified differential equations. Thus, not only the true part of the solution, but also the parasitic parts are asymptotically governed by differential equations, and an asymptotic analysis based on theory for differential equations can be developed. However, before this kind of analysis can be applied to preconditioning techniques, we have to extend the theory to partial differential equations.

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