IMPLICIT-EXPLICIT METHODS FOR TIME-DEPENDENT PDE'S

By

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BMATH, University of Waterloo, 1991

A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF
THE REQUIREMENTS FOR THE DEGREE OF
MASTER OF SCIENCE

in
THE FACULTY OF GRADUATE STUDIES
DEPARTMENT OF MATHEMATICS
AND
INSTITUTE OF APPLIED MATHEMATICS

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April 1993
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Abstract

Various methods have been proposed to integrate dynamical systems arising from spatially discretized time-dependent partial differential equations. For problems with terms of different types, implicit-explicit (IMEX) schemes have been used, especially in conjunction with spectral methods. For convection-diffusion problems, for example, one would use an explicit scheme for the convection term and an implicit scheme for the diffusion term. Reaction-diffusion problems can also be approximated in this manner. In this work we systematically analyze the performance of such schemes, propose improved new schemes and pay particular attention to their relative performance in the context of fast multigrid algorithms and aliasing reduction for spectral methods.

For the prototype linear advection-diffusion equation, a stability analysis for first, second, third and fourth order multistep IMEX schemes is performed. Stable schemes permitting large time steps for a wide variety of problems and yielding appropriate decay of high frequency error modes are identified.

Numerical experiments demonstrate that weak decay of high frequency modes can lead to extra iterations on the finest grid when using multigrid computations with finite difference spatial discretization, and to aliasing when using spectral collocation for spatial discretization. When this behaviour occurs, use of weakly damping schemes such as the popular combination of Crank-Nicolson with second order Adams-Bashforth is discouraged and better alternatives are proposed.

Our findings are demonstrated on several examples.
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Acknowledgements

First and foremost, many thanks to my supervisors Dr. Uri Ascher and Dr. Brian Wetton for their many helpful suggestions while working on this thesis. I would also like to thank NSERC for financially supporting me during my graduate work.
Chapter 1

Introduction

1.1 IMEX Schemes

This thesis considers multistep methods for computing approximate solutions to large systems of ordinary differential equations which arise from the spatial discretization of time-dependent partial differential equations. Such systems typically have the form

\[ \dot{u} = f(u) + \nu g(u) \]  

(1.1)

where \( \|g\| \) is normalized and \( \nu \) is a nonnegative parameter.

The term \( f(u) \) in (1.1) is some possibly nonlinear term which we do not want to integrate implicitly. This could be because the Jacobian of \( f(u) \) is non-symmetric and non-definite and an iterative solution of the implicit equations is desired, or the Jacobian could be dense, as in spectral methods, requiring the inversion of a full matrix at each time step. One may simply wish to integrate \( f(u) \) explicitly for ease of implementation. The term \( \nu g(u) \), however, is a stiff term which should be integrated implicitly to avoid excessively small time steps. Frequently \( \nu g(u) \) is a linear diffusion term, in which case the implicit equations form a linear system which is positive definite, symmetric and sparse. Such systems can be solved efficiently by iterative techniques (see Varga[23] or Hackbusch[10]). Thus for problems of the form (1.1) it often makes sense to integrate \( \nu g(u) \) implicitly and \( f(u) \) explicitly. Such implicit-explicit methods will be referred to as IMEX schemes.
Problems of the form (1.1) frequently occur in practice. For example, convection-diffusion problems lead to such systems. Kim and Moin[13], for instance, applied a projection scheme to the incompressible Navier-Stokes equations to obtain a nonlinear convection-diffusion problem to solve at each time step. This system was solved using second order Adams-Bashforth for the convection term and Crank-Nicolson for the diffusion term. Applied to (1.1) this popular scheme gives

\[
\frac{u^{n+1} - u^n}{k} = \frac{3}{2} f(u^n) - \frac{1}{2} f(u^{n-1}) + \frac{\nu}{2} [g(u^{n+1}) + g(u^n)]
\]  

(1.2)

where \(k\) is the constant discretization step size and \(u^n\) is the numerical approximation to \(u(kn)\).

A wide variety of other applications for IMEX schemes are also possible. For example, solutions to reaction-diffusion systems arising in chemistry and mathematical biology can be computed using this technique. For these problems the nonlinear reaction term can be treated explicitly while the diffusion term is treated implicitly. Examples of reaction-diffusion systems from a biological standpoint can be found in Murray[16].

Several authors have analyzed specific IMEX schemes. For example, an experimental analysis of several implicit-explicit schemes including (1.2) was carried out by Basdevant et al.[1]. Varah[22] determines some stability properties for certain second order IMEX schemes. These studies do not address how to choose the best IMEX scheme for a given system (1.1). This thesis seeks efficient IMEX schemes for convection-diffusion and reaction-diffusion problems by systematically examining the stability properties of the linearized systems and performing numerical experiments.

Methods which allow the largest stable time steps are sought. In particular, for \(\nu \gg 1\) we seek methods possessing a mild time step restriction since the system (1.1) is dominated by the implicitly handled "diffusion term". For other values of \(\nu \geq 0\) we seek schemes which have reasonable time-stepping restrictions. A restriction similar to the
Chapter 1. Introduction

Courant-Friedrich-Lewy (CFL) condition is reasonable because this guarantees that the domain of dependence of the scheme includes the domain of dependence of the differential equation for explicit schemes applied to the one-dimensional wave equation, \( u_t = au_x \) (see Strikwerda[19]).

Strong decay of high frequency spatial modes is another property which is important in many applications. Schemes which possess this property are identified and compared to standard schemes such as (1.2). As discussed in the next two sections, this property has important implications for the efficiency of time-dependent multigrid and pseudospectral computations.

1.2 Multigrid and IMEX Schemes

As mentioned in the previous section, IMEX schemes typically generate at each time step implicit systems represented by sparse, symmetric, positive definite matrices. In two or higher dimensions, iterative techniques are particularly suitable for solving such systems. A multigrid solution for the implicit equations may be especially attractive because only \( \mathcal{O}(N) \) floating point operations are ideally needed for solving simple steady state problems, where \( N \) is the size of the ODE system (1.1) arising from \( N \) spatial grid points (see Hackbusch[10]).

In many physical problems with diffusion, high frequency solution components dissipate quickly. For multigrid this is a desirable property for the numerical solution since it may reduce the number of costly iterations on the finest grid. Brandt and Greenwald[5] argue that non-physical high frequency components are especially harmful when applying red-black Gauss-Seidel relaxation. This is because this smoothing technique aliases high frequency errors into low frequency components which linger on for many time steps. Nonetheless, red-black Gauss-Seidel relaxation is often used, since it has a very good
smoothing rate and it is parallelizable.

Several useful suggestions have been made by Brandt and Greenwald[5] to address these problems. One of these is use of a double discretization technique. This method uses Backward Euler during relaxation sweeps and Crank-Nicolson for calculating transferred residuals. We do not consider this technique because it may be fragile in applications since high frequency components must be damped very strongly to obtain second order accuracy using a first order scheme for relaxation sweeps.

Brandt and Greenwald[5] recommend use of W-cycles instead of V-cycles to help remove aliased low frequency components from coarser grids. W-cycles are more expensive than V-cycles, however. Furthermore, this method does nothing to remove non-physical high frequencies on the finest grid.

They further propose to avoid the final smoothing pass at each time step. This may reduce low frequency aliasing errors since it ensures that all relaxations are followed by a coarse grid correction. However, this idea also does not eliminate non-physical high frequency components on the finest grid.

Finally, Brandt and Greenwald[5] suggest a modified FMG algorithm where the first coarse grid correction is performed before iterating on the finest grid. This should produce the maximum effect from relaxation since the increment between time steps is generally smooth. In Chapter 4, however, numerical experiments for the 2D convection-diffusion problem demonstrate that this method alone can be inefficient for eliminating non-physical high frequency components.

This thesis proposes use of a highly damping time-stepping method to control non-physical high frequency spatial components. This technique produces little or no additional expense because strongly damping time-stepping schemes require approximately the same number of floating point operations as standard schemes such as (1.2). In Chapter 4, highly damping IMEX schemes are compared experimentally to standard schemes
to verify that these methods are very effective for reducing the number of iterations on the finest grid, thus providing a more efficient multigrid method for time-dependent problems.

1.3 Spectral Methods and IMEX Schemes

As mentioned in Section 1.1, IMEX schemes are frequently used in spectral methods. Fully implicit schemes are impractical because a dense system originating from the convection term must be solved at each time step. Explicit schemes are usually avoided because they frequently require unreasonably small time steps to ensure stability. The time step restriction for a Chebyshev basis (see Canuto et al.[6]) is particularly severe. For this basis, the one-dimensional heat equation with Dirichlet or Neumann boundary conditions, for example, requires the time step restriction $k = \mathcal{O}(N^{-4})$ as $N \to \infty$ where $N$ is the number of basis functions. This result follows from the fact that the largest eigenvalue, $\lambda$, has magnitude $|\lambda| = \mathcal{O}(N^4)$ as $N \to \infty$ (see Canuto et al.[6]). For further information about spectral methods applied to fluids and other problems see Canuto et al.[6] or Boyd[2].

It is known that aliasing effects can complicate solutions for pseudospectral methods (see Canuto et al.[6]). These effects occur when nonlinear terms produce high frequencies that cannot be represented in the basis and thus contribute erroneously to low frequencies. Since only the highest frequencies alias into low frequencies we expect that a weak decay of high frequency spatial modes will contribute excessively to aliasing effects.

Several methods have been proposed to deal with this behaviour. One such method is the 3/2’s rule (see Canuto et al.[6]). Using this technique, a quadratically nonlinear term is computed using $3N/2$ basis functions. At the end of the calculation, coefficients for the basis functions representing the $N$ lowest frequencies are kept. Only $3N/2$ basis functions
are required since frequencies which cannot be represented in the basis contribute to frequencies that are later neglected. An alternative to the $3/2$'s rule is the $2/3$'s rule. For this method, the highest $1/3$ frequencies are eliminated before any aliasing calculation. These methods eliminate aliasing but the $3/2$'s rule requires approximately 50% more floating point operations than an aliased computation (see Canuto et al.[6]), while the $2/3$'s rule causes a dramatic loss of high frequency information at each time step. Other methods (see Canuto et al.[6]) such as applying a finer spatial mesh or using phase shifts also necessitate extra work.

We propose to reduce aliasing by using a highly damping time-stepping method. In Chapter 4, numerical experiments are performed to compare highly damping schemes to standard schemes such as (1.2). These computations demonstrate that this inexpensive method of reducing aliasing can be very effective in aliased pseudospectral computations.

1.4 Overview

In Chapter 2, general linear multistep IMEX schemes are defined, and the optimal accuracy for such schemes is derived. This is followed by a description of characteristic polynomials and other aspects of the stability theory used for analyzing properties of multistep schemes. First and second order schemes are discussed. In particular, parameterizations for first and second order schemes are given. For the linear advection-diffusion equation, stability properties for several popular methods are determined and stability for $\nu = 0$ is considered. High frequency modal decay and time step restrictions for second order schemes are studied in detail to determine the optimal method for various problems.

In Chapter 3, third and fourth order IMEX schemes are discussed. A parameterization for third order schemes is given and the method with the strongest high frequency decay
is identified. The stability properties for several methods are compared for $\nu \gg 1$ and $\nu = 0$. A fourth order scheme is defined and several of its stability properties are derived for $\nu \gg 1$ and $\nu = 0$. This chapter concludes with a comparison of second, third and fourth order IMEX schemes.

In Chapter 4, numerical experiments for convection-diffusion problems are carried out. For the finite difference case, solutions to variable coefficient and nonlinear problems are computed to support the stability results of Chapter 2. Some properties of IMEX schemes in pseudospectral methods are also demonstrated for the Burgers equation. In particular, these computations show that the use of strongly damping time-stepping schemes reduces aliasing inexpensively and effectively. By computing the solutions to the 2D convection-diffusion equation using finite differences, it is also shown that the use of a strongly damping time-stepping scheme can give a more efficient multigrid method for time-dependent problems. This chapter concludes by discussing how to choose IMEX schemes for arbitrary convection-diffusion problems.

In Chapter 5, the application of IMEX schemes to reaction-diffusion systems is considered. A description of the two chemical reaction-diffusion problem is given and a linear analysis of this problem is carried out to determine how it differs from the convection-diffusion problem. Based on this analysis and experimental evidence, efficient IMEX schemes are determined. This chapter concludes by describing how to choose IMEX schemes for reaction-diffusion problems.

Conclusions are presented in Chapter 6. Suggestions as to the direction of future research are also proposed.
Chapter 2

First and Second Order IMEX Schemes

Properties of general linear multistep IMEX schemes for the system of ordinary differential equations

\[ \dot{u} = f(u) + \nu g(u) \]  

(2.3)

are derived in the first four sections of this chapter. Subsequent sections determine stability properties of first and second order IMEX schemes for the one-dimensional linear advection-diffusion equation. These results are compared to numerical experiments of more complicated examples in Chapters 4 and 5.

2.1 General Linear Multistep IMEX Schemes

We now derive \( s \)-step IMEX schemes for (2.3), \( s \geq 1 \). Letting \( k \) be the discretization step size and \( u^n \) denote the approximate solution at \( t_n = kn \), these schemes may be written,

\[ \frac{1}{k} u^{n+1} + \frac{1}{k} \sum_{j=0}^{s-1} a_j u^{n-j} = \sum_{j=0}^{s-1} b_j f(u^{n-j}) + \nu \sum_{j=-1}^{s-1} c_j g(u^{n-j}) \]  

(2.4)

where \( c_{-1} \neq 0 \). For a smooth function \( u(t) \), expand (2.4) in a Taylor series about \( t_n = n\Delta t \) to obtain the truncation error. This yields

\[ \frac{1}{k} \left[ 1 + \sum_{j=0}^{s-1} a_j u(t_n) \right] + \left[ 1 - \sum_{j=1}^{s-1} j a_j \right] \dot{u}(t_n) + \cdots + \frac{k^{p-1}}{p!} \left[ 1 + \sum_{j=1}^{s-1} (-j)^p a_j \right] u(p)(t_n) \]

\[ - \sum_{j=0}^{s-1} b_j f(u(t_n)) + k \sum_{j=1}^{s-1} j b_j \frac{df}{dt} \bigg|_{t=t_n} - \cdots - \frac{k^{p-1}}{(p-1)!} \sum_{j=1}^{s-1} (-j)^{p-1} b_j \frac{d^{p-1}f}{dt^{p-1}} \bigg|_{t=t_n} \]

\[ -\nu \sum_{j=-1}^{s-1} c_j g(u(t_n)) - k\nu [c_{-1} - \sum_{j=-1}^{s-1} c_j] \frac{dg}{dt} \bigg|_{t=t_n} - \cdots \]
\[ -\frac{k^{p-1}}{(p-1)!} \nu [c_{-1} + \sum_{j=1}^{s-1} c_j (-j)^{p-1} \frac{d^{p-1} g_i}{dt^{p-1}}] \big|_{t=t_n} + \mathcal{O}(k^p). \] (2.5)

Applying Equation (2.3) to the truncation error (2.5), an order \( p \) scheme is obtained provided

\[
\begin{align*}
1 + \sum_{j=0}^{s-1} a_j &= 0 \\
1 - \sum_{j=1}^{s-1} ja_j &= \sum_{j=0}^{s-1} b_j = \sum_{j=-1}^{s-1} c_j \\
1 + \sum_{j=1}^{s-1} \frac{j^2}{2} a_j &= -\sum_{j=1}^{s-1} j b_j = c_{-1} - \sum_{j=1}^{s-1} j c_j \\
&\vdots \\
\frac{1}{p!} + \sum_{j=1}^{s-1} \frac{(-j)^{p-1} b_j}{p!} a_j &= \sum_{j=1}^{s-1} \frac{(-j)^{p-1} c_j}{(p-1)!} = \frac{c_{-1}}{(p-1)!} + \sum_{j=1}^{s-1} \frac{(-j)^{p-1} c_j}{(p-1)!}.
\end{align*}
\] (2.6)

Having determined constraints (2.6) for an order \( p \), \( s \)-step IMEX scheme, we next examine how to select \( p \) for a given \( s \).

### 2.2 Optimal Accuracy for IMEX Schemes

We begin by showing that the \((2p+1)\) constraints of system (2.6) are linearly independent provided \( p \leq s \). Because linear independence for \( p = s \) implies linear independence for \( p \leq s \), we need only consider the case \( p = s \).

The coefficient matrix for \([a_0, \cdots a_{s-1}, b_0, \cdots b_{s-1}, c_{-1}, \cdots c_{s-1}]^T\) representing the system (2.6) is

\[
\begin{bmatrix}
A_s & 0 & \cdots & 0 \\
0 & (-1)^s \cdots (1-s)^s & -D_s A_s \\
0 & -A_s & \ddots & A_s \\
& & & 1
\end{bmatrix}
\] (2.7)
where $A_s$ and $D_s$ are $s \times s$ matrices,

$$A_s = \begin{bmatrix}
1 & 1 & 1 & \cdots & 1 \\
0 & -1 & -2 & \cdots & 1 - s \\
0 & 1 & 4 & \cdots & (1 - s)^2 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & (-1)^{s-1} & (-2)^{s-1} & \cdots & (1 - s)^{s-1}
\end{bmatrix}$$

and

$$D_s = \begin{bmatrix}
1 \\
2 \\
\vdots \\
s
\end{bmatrix}.$$

The matrix $A_s$ is nonsingular. To see this, note that it is a Vandermonde matrix based on the distinct values $0, -1, -2, \ldots, 1 - s$, and as such is nonsingular (see Golub and Van Loan[9]).

Because $A_s$ is nonsingular, it is easy to see that columns $1, s+1, \ldots, 2s, 2s+2, \ldots, 3s+1$ of matrix (2.7) are linearly independent. Thus all $(2p + 1)$ constraints are linearly independent and system (2.6) must admit a $(3s - 2p)$ parameter family of solutions for $p \leq s$. Since column $(2s + 1)$ of matrix (2.7) does not figure into the above proof we know $c_{-1}$ can have any nonzero value. This property verifies that the family of schemes is IMEX.

We next verify that an $s$-step IMEX scheme cannot have accuracy greater than $O(k^s)$. Any $O(k^{s+r})$ scheme using $s$ levels, $r \geq 1$, must satisfy the following constraints,

$$\sum_{j=0}^{s-1} b_j = \sum_{j=1}^{s-1} c_j$$

$$\sum_{j=1}^{s-1} (-j)b_j = c_{-1} + \sum_{j=1}^{s-1} (-j)c_j$$
\[ \sum_{j=1}^{s-1} (-j)^s b_j = c_{-1} + \sum_{j=1}^{s-1} (-j)^s c_j \]  
\tag{2.8}

Letting \( \mu_j = c_j - b_j \) the system (2.8) yields,
\[ c_{-1} + \sum_{j=0}^{s-1} \mu_j = 0 \]
\[ c_{-1} + \sum_{j=1}^{s-1} \mu_j (-j) = 0 \]
\[ \vdots \]
\[ c_{-1} + \sum_{j=1}^{s-1} \mu_j (-j)^s = 0 \]  
\tag{2.9}

Similar to the preceding proof the coefficient matrix for (2.9),
\[
B \equiv \begin{bmatrix}
1 & 1 & 1 & \cdots & 1 \\
1 & 0 & -1 & \cdots & -(s-1) \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
1 & 0 & (-1)^s & \cdots & (1-s)^s \\
\end{bmatrix}
\]

is nonsingular and so
\[ B \begin{bmatrix}
c_{-1} \\
\mu_0 \\
\vdots \\
\mu_{s-1} \\
\end{bmatrix} = 0 \]

implies that \( c_{-1} = 0 \) and \( b_j = c_j, j = 1, \ldots, s-1 \). Since an IMEX scheme requires that \( c_{-1} \neq 0 \), an \( s \)-step IMEX scheme is unable to achieve more than order \( s \) accuracy.

Because it is desirable to achieve the greatest accuracy with the fewest steps, the remainder of this work only considers \( s \)-step, \( O(k^s) \) schemes. As shown above, the family of such schemes has exactly \( s \) free parameters.
2.3 Method of Analysis

All the IMEX methods (2.4) are consistent, provided the constraints (2.6) are satisfied. By the Lax-Richtmeyer Theorem (see Strikwerda[19]), these methods also are convergent when applied to a well-posed initial value problem, provided stability is ensured.

General, sufficient stability criteria are difficult to specify because the ODE system (2.4) is potentially very large. To derive stability properties of IMEX methods, we consider the one-dimensional advection-diffusion equation, \( U_t = aU_x + \nu U_{xx} \) where \( a \) and \( \nu \) are constants, \( \nu > 0 \), subject to periodic boundary conditions. Properties derived from the analysis of this simple prototype problem should provide clues to the behaviour of discretizations of more complicated parabolic-hyperbolic systems.

Using centred approximations, \( D_1 \) and \( D_2 \), for the first and second derivatives, respectively, we obtain the corresponding semi-discrete equations.

\[
\dot{U}_i = a D_1 U_i + \nu D_2 U_i, 1 \leq i \leq M.
\]

(Here, a uniform spatial grid with \( M \) points has been employed.) Applying a discrete Fourier transform diagonalizes this system to

\[
\dot{x}_j = i\beta_j x_j + \alpha_j x_j, j = 1 \ldots M
\]

where \( \alpha_j \) and \( \beta_j \) are given in (2.13) below. For notational convenience, we write

\[
\dot{x} = i\beta x + \alpha x.
\]  

(2.10)

Applying the general multistep IMEX scheme (2.4) to (2.10) yields

\[
\frac{1}{k} x^{n+1} + \frac{1}{k} \sum_{j=0}^{s-1} a_j x^{n-j} = \sum_{j=0}^{s-1} b_j i\beta x^{n-j} + \sum_{j=-1}^{s-1} c_j \alpha x^{n-j}
\]  

(2.11)

which is a linear difference equation with constant coefficients. (In comparing (2.11) to (2.4) note that \( \nu \) is buried in \( \alpha \).) The solutions of Equation (2.11) are of the form

\[
x^{n+1} = p_1 \tau_1^n + p_2 \tau_2^n + \cdots + p_s \tau_s^n
\]
Chapter 2. First and Second Order IMEX Schemes

Figure 2.1: Half Ellipse of Possible ($\alpha, \beta$)

where $\tau_j$ is the $j^{th}$ root of the characteristic equation defined by

$$\Phi(z) \equiv (1 - c_{-1} \alpha k)z^s + \sum_{j=0}^{s-1}(a_j - b_j \beta k - c_j \alpha k)z^{s-j-1}$$  \hspace{1cm} (2.12)

and $p_j$ is constant for $\tau_j$ simple and a polynomial in $n$ otherwise. Clearly, stability holds for $|\tau_j| \leq 1$, $\tau_j$ simple and $|\tau_j| < 1$ where $\tau_j$ is a multiple root.

Throughout this thesis, we consider $D_1$ and $D_2$ such that $D_1 U_i = \frac{U_{i+1} - U_{i-1}}{2h}$ and $D_2 U_i = \frac{U_{i+1} - 2U_i + U_{i-1}}{h^2}$. This determines that

$$(\alpha_j, \beta_j) = \left(\frac{2\nu}{h^2}[\cos(2\pi j h) - 1], \frac{a}{h} \sin(2\pi j h)\right)$$ \hspace{1cm} (2.13)

which lie on the ellipse of Figure 2.1. Determination of time-stepping restrictions is accomplished by finding the largest time step such that the ellipse lies in the absolute stability region of the IMEX scheme.

Another important property can also be examined using these techniques. From the exact solution of $\dot{x} = i \beta x + \alpha x$ it follows that $|x(t_{n+1})| = e^{\alpha t}|x(t_n)|$. Thus the
amplification associated with the differential equation (2.10) over a time interval of length $k$ is given by $e^{\alpha k}$. The corresponding contours in the $\alpha$-$\beta$ plane are plotted in Figure 2.2. From this figure, we note that, ideally, the roots of the characteristic polynomial for our method should be small for $\alpha$ large and negative. This behavior corresponds to fast decay of high frequency components when $\nu$ is large. As discussed in Sections 1.2 and 1.3, this behaviour often is particularly desirable when applying spectral collocation to an aliased computation or if a multigrid method is contemplated for the solution of the implicit equations.

2.4 Schur and von Neumann Polynomials

From the previous section we see that stability results for IMEX schemes are obtained by examining the roots of the characteristic equation (2.12). To obtain results for the $\beta$-axis for the higher order schemes considered in Chapter 3 we use the theory of Schur and von Neumann polynomials (see Miller[14]). The relevant definitions and theorems
from the discussion in Sections 4.2 and 4.3 of Strikwerda[19] are outlined below.

Definition 2.4.1 The polynomial $\varphi$ is a Schur polynomial if all its roots, $\tau_j$ satisfy $|\tau_j| < 1$.

Definition 2.4.2 The polynomial $\varphi$ is a von Neumann polynomial if all its roots, $\tau_j$ satisfy $|\tau_j| \leq 1$.

Definition 2.4.3 The polynomial $\varphi$ is a simple von Neumann polynomial if $\varphi$ is a von Neumann polynomial and its roots on the unit circle are simple roots.

Definition 2.4.4 For any polynomial $\varphi = \sum_{i=0}^{d} a_i z^i$ the polynomial $\varphi^*$ is defined by $\varphi^* = \sum_{i=0}^{d} \bar{a}_{-i} z^i$, where $\bar{a}$ denotes the complex conjugate of $a$.

Definition 2.4.5 For any polynomial $\varphi_0(z)$ we define recursively the polynomial $\varphi_{j+1}(z) = \frac{\varphi_j'(0)\varphi_j(z) - \varphi_j(0)\varphi_j'(z)}{z}$.

Theorem 2.4.1 $\varphi_j$ is a simple von Neumann polynomial if and only if either $|\varphi_j'(0)| < |\varphi_j'(0)|$ and $\varphi_j$ is a simple von Neumann polynomial or $\varphi_{j+1}$ is identically zero and $\varphi_j'$ is a Schur polynomial.

Theorem 2.4.2 A necessary condition for the finite difference scheme to be stable is that the characteristic polynomial $\Phi$ defined in (2.12) is a simple von Neumann polynomial.

2.5 First Order IMEX Schemes

We proceed by deriving one-step, first order IMEX schemes for Equation (2.3). One representation of this one-parameter family of schemes yields,

$$u^{n+1} - u^n = kf(u^n) + \nu k[(1 - \gamma)g(u^n) + \gamma g(u^{n+1})]$$

(2.14)
and we restrict \( 0 \leq \gamma \leq 1 \) to prevent large truncation error. As we have shown in Section 2.2, this one-parameter family must describe all first order, one-step IMEX schemes.

Some of these schemes are familiar. For example, the choice \( \gamma = 0 \) yields the Forward Euler scheme,

\[
u^{n+1} - u^n = kf(u^n) + \nu kg(u^n).
\]

This scheme is fully explicit, and will not be considered further.

Another possibility is to apply Backward Euler to \( g \) and Forward Euler to \( f \). This choice \( (\gamma = 1) \) yields,

\[
u^{n+1} - u^n = kf(u^n) + \nu kg(u^{n+1}). \tag{2.15}
\]

Backward Euler is the first order member of the class of backward differencing formulas (BDF's) (see Gear[8]). These implicit schemes are centred in time about time step \((n+1)\). Implicit-explicit methods such as (2.15) which apply a BDF to \( g \) and which extrapolate \( f \) to time step \((n+1)\) will be referred to as semi-implicit BDF (SBDF) schemes.

Having determined integration formulae, we next consider stability properties for first order IMEX schemes.

### 2.6 Stability of First Order IMEX Schemes

From Equation (2.14) the general first order IMEX scheme applied to \( \dot{x} = (\alpha + i\beta)x \) is

\[
x^{n+1} = \xi(\alpha, \beta)x^n
\]

where

\[
\xi(\alpha, \beta) = \frac{1 + k\alpha(1 - \gamma) + ik\beta}{1 - k\gamma \alpha}.
\]

The stability region is thus \( \lbrace (\alpha, \beta) : |\xi(\alpha, \beta)| \leq 1 \rbrace \).

Figure 2.3 presents stability contours for first order SBDF, \( \gamma = 1 \). Strong decay occurs for \( \alpha \) large and negative. Furthermore, the scheme allows variable time-stepping and uses relatively little storage. For first order schemes, the choice \( \gamma = 1 \) is often preferred since
smaller \( \gamma \) values do not have as good decay properties and may become marginally stable or unstable for large \( \nu \). See Figure 2.4 for the case \( \gamma = \frac{1}{2} \), which yields the second order Crank-Nicolson scheme when \( f \equiv 0 \).

All first order IMEX schemes have the shortcoming that they are unstable for \( \nu = 0, \alpha \neq 0 \), since

\[
|\xi(0, \beta)| = |1 + ik\beta| = \sqrt{1 + k^2\beta^2} > 1.
\]

Furthermore, at least a second order time-stepping scheme is often desirable since a second order spatial discretization is used. We thus consider second order methods for the remainder of this chapter.

### 2.7 Second Order IMEX Schemes

Approximating \( \dot{u} = f(u) + \nu g(u) \) to second order using IMEX schemes leaves two free parameters. If we centre our schemes in time about time step \( (n + \gamma) \) to second order,
we obtain the following family,

\[
\frac{1}{k}[(\gamma + \frac{1}{2})u^{n+1} - 2\gamma u^n + (\gamma - \frac{1}{2})u^{n-1}] =
(\gamma + 1)f(u^n) - \gamma f(u^{n-1}) + 
\nu[(\gamma + \frac{c}{2})g(u^{n+1}) + (1 - \gamma - c)g(u^n) + \frac{c}{2}g(u^{n-1})].
\quad (2.16)
\]

Some of these methods are quite familiar. For example, selecting \((\gamma, c) = (\frac{1}{2}, 0)\) yields

\[
\frac{1}{k}[u^{n+1} - u^n] = \frac{3}{2}f(u^n) - \frac{1}{2}f(u^{n-1}) + \nu[\frac{9}{16}g(u^{n+1}) + \frac{3}{8}g(u^n) + \frac{1}{16}g(u^{n-1})]
\quad (2.17)
\]

which is one of the more frequently used schemes in spectral methods applications (e.g. Canuto et al.[6] and Kim and Moin[13]). Because it applies Crank-Nicolson for the implicit part and second order Adams-Bashforth for the explicit part, this scheme will be referred to as CNAB (Crank-Nicolson, Adams-Bashforth). In the next section, we show that the best asymptotic decay properties for \(\gamma = \frac{1}{2}\) occur when \(c = \frac{1}{8}\). This choice gives

\[
\frac{1}{k}[u^{n+1} - u^n] = \frac{3}{2}f(u^n) - \frac{1}{2}f(u^{n-1}) + \nu[\frac{9}{16}g(u^{n+1}) + \frac{3}{8}g(u^n) + \frac{1}{16}g(u^{n-1})]
\quad (2.18)
\]
Because of the obvious similarity to CNAB, this scheme will be called modified CNAB.

By setting $(\gamma, c) = (0, 1)$ in (2.16) we obtain another method which has been applied to spectral applications (e.g. Brachet et al.[3]),

$$\frac{1}{2k}[u^{n+1} - u^{n-1}] = f(u^n) + \frac{\nu}{2}[g(u^{n+1}) + g(u^{n-1})].$$  \hfill (2.19)

This scheme uses leap frog explicitly and something similar to Crank-Nicolson implicitly. For this reason, this method shall be referred to as CNLF (Crank-Nicolson, Leap Frog).

Finally, setting $(\gamma, c) = (1, 0)$ yields

$$\frac{1}{2k}[3u^{n+1} - 4u^n + u^{n-1}] = 2f(u^n) - f(u^{n-1}) + \nu g(u^{n+1})$$  \hfill (2.20)

which shall be referred to as SBDF since this scheme is centred about time step $(n + 1)$. Other authors, such as Varah[22], call this scheme extrapolated Gear.

Having determined integration formulae, we direct our attention to obtaining stability properties for second order IMEX schemes.

### 2.8 Choice of $c$ for Second Order Schemes

The second degree characteristic polynomial resulting from (2.16) applied to $\dot{x} = (\alpha + i\beta)x$ is given by

$$\Phi(z) = [\gamma + \frac{1}{2} - \alpha k(\gamma +\frac{c}{2})]z^2 - [2\gamma + i\beta k(\gamma + 1) + \alpha k(1 - \gamma - c)]z + \gamma - \frac{1}{2} + i\beta k\gamma - \alpha k\frac{c}{2}$$  \hfill (2.21)

Because the parameter $c$ in Equation (2.21) is always multiplied by $\alpha$ we choose $c$ according to stability properties for $|\alpha| \gg 1/k$. For this case, the roots of the characteristic equation (2.21) are given approximately by

$$(\gamma + \frac{c}{2})\tau^2 + (1 - \gamma - c)\tau + \frac{c}{2} = 0$$
which gives us

$$\tau_{1,2} = \frac{\gamma + c - 1 \pm \sqrt{(1 - \gamma)^2 - 2c}}{2\gamma + c}.$$ 

For any \((\gamma, c)\), evaluating

$$D_{\gamma,c} \equiv \max(|\tau_1|, |\tau_2|)$$

provides an estimate of the high frequency modal decay for large \(\nu\). Minimization over \(c\) determines the method with the strongest asymptotic high frequency decay for a particular \(\gamma\).

First consider \(c \leq \frac{(1 - \gamma)^2}{2}\). Using elementary calculus, it is easy to verify that

$$\min_{c \leq \frac{(1 - \gamma)^2}{2}} \frac{\sqrt{(1 - \gamma)^2 - 2c}}{2\gamma + c}$$

and

$$\min_{c \leq \frac{(1 - \gamma)^2}{2}} \frac{\gamma + c - 1}{2\gamma + c}$$

occur when \(c = \frac{(1 - \gamma)^2}{2}\). Thus the minimum for \(D_{\gamma,c}\) must occur when \(c \geq \frac{(1 - \gamma)^2}{2}\). For \(c \geq \frac{(1 - \gamma)^2}{2}\) we have

$$\min_{c \geq \frac{(1 - \gamma)^2}{2}} D_{\gamma,c} = \min_{c \geq \frac{(1 - \gamma)^2}{2}} \frac{c}{2\gamma + c} = \frac{1 - \gamma}{1 + \gamma}.$$ (2.23)

From which it is clear that the minimum is attained for \(c = \frac{(1 - \gamma)^2}{2}\) if \(\gamma > 0\) and \(c \geq \frac{1}{2}\) if \(\gamma = 0\).

In subsequent sections we use the following simple estimates of the high frequency decay:

$$D_{\gamma,0} = \frac{1 - \gamma}{\gamma},$$

$$D_{\gamma,1-\gamma} = \sqrt{\frac{1 - \gamma}{1 + \gamma}},$$

$$D_{\gamma,\frac{(1 - \gamma)^2}{2}} = \frac{1 - \gamma}{\gamma + 1}.$$
These results show that for \( c = 0 \), we need \( \gamma \geq \frac{1}{2} \) to ensure stability for all \( \nu \). Furthermore, from Equation (2.23), \( D_{\gamma,c} = 0 \iff (\gamma, c) = (1, 0) \) which implies that SBDF possesses the strongest asymptotic decay of second order methods.

### 2.9 Second Order Instability along the Nonzero \( \beta \)-Axis

We proceed by verifying stability at the origin, \((\alpha, \beta) = (0,0)\). At the origin, the roots of the characteristic equation (2.21) are 1 and \( \frac{\gamma - 1}{\gamma + 1} \). These are simple roots, whose magnitude does not exceed 1 provided \( \gamma \geq 0 \). Thus by Theorem (2.4.2), \((\alpha, \beta) = (0,0)\) is stable for all second order IMEX schemes such that \( \gamma \geq 0 \).

Stability along the \( \beta \)-axis is also a desirable characteristic. Schemes which exhibit this behaviour are better able to compute solutions for problems with very small \( \nu \) and for convection problems with small artificial diffusion. For this reason, the remainder of this section considers second order methods applied to the one-dimensional wave equation, \( \dot{x} = i\beta x \).

Applying a second order IMEX scheme such that \( \gamma = 0 \) to the problem \( \dot{x} = i\beta x \) yields the leap frog scheme. Leap frog is known to be stable when applied to \( \dot{x} = i\beta x \), provided \( k < \frac{\hbar}{a} \), as is outlined in many texts such as Strikwerda[19]. Thus the CNLF scheme, in particular, is stable on the \( \beta \)-axis provided \( k < \frac{\hbar}{a} \).

For other IMEX schemes, we know from Varah[22] that when \( \alpha = 0 \) one of the roots, \( \tau_i \), of Equation (2.21) satisfies

\[
|\tau_i(\beta k)|^2 = 1 + (\gamma^2 + \frac{\gamma}{2})(\beta k)^4 + \cdots > 1
\]

for \( \beta k \) sufficiently small and \( \gamma > 0 \). Thus for all \( k \), all second order schemes such that \( \gamma > 0 \) are unstable on the nonzero \( \beta \)-axis.
2.10 Second Order Stability Contours

Further information can be obtained from the stability contours in the $\alpha - \beta$ plane. These plots are displayed in Figures 2.5 to 2.10. Figure 2.5 shows the contours for CNLF. This method is stable for all $\nu \geq 0$, provided $k < \frac{h}{a}$. Such a time step restriction is undesirable since it applies even for large $\nu$ and small $h$. Furthermore, the decay of high frequency modes can be weak, tending to 1 as $\alpha$ tends to $-\infty$. Comparison of CNLF to other second order methods such that $\gamma = 0$ suggests that CNLF produces the largest stability region among such methods.

The contours for CNAB are plotted in Figure 2.6. This method has a reasonable time step restriction for larger $\nu$ and small $h$. It is unstable near the $\beta$-axis, however. It also suffers from poor decay of high frequency modes, since the decay tends to 1 as $\alpha$ tends to $-\infty$. Using modified CNAB, $(\gamma, c) = (\frac{1}{2}, \frac{1}{8})$, the decay tends to $\frac{1}{3}$, a significant improvement. See Figure 2.7 for these contours.
Figure 2.6: Stability Contours for CNAB, $(\gamma, c) = (\frac{1}{2}, 0)$

Figure 2.7: Stability Contours for Modified CNAB, $(\gamma, c) = (\frac{1}{2}, \frac{1}{8})$
Chapter 2. First and Second Order IMEX Schemes

Figure 2.8: Stability Contours for SBDF, $(\gamma, c) = (1, 0)$

The contours for SBDF are displayed in Figure 2.8. This method has the mildest time-stepping restriction when $\nu$ is large and $h$ is small. The decay of high frequency modes is strong, tending to 0 as $\alpha$ tends to $-\infty$. This method, however, has the strictest time step limitation for small $|\alpha|$.

For $\gamma = .25$, stability contours for $c = \frac{(1-\gamma)^2}{2} = .28125$ and $c = (1-\gamma) = .75$ are plotted in Figures 2.9 and 2.10. Comparison of these contours indicates that $c = (1-\gamma) = .75$ possesses a milder time step restriction for large $\nu$. Thus the method with the strongest asymptotic decay does not necessarily allow the largest stable time steps when $\nu$ is large.

Many other methods can be considered. The next section discusses which second order method allows the largest stable time steps for a particular problem.

2.11 Choice of Second Order Method

We now develop a quantitative method for describing time step restrictions for second order schemes. Such a method will help select which second order scheme to use for a
Figure 2.9: Stability Contours for $(\gamma, c) = (0.25, 0.28125)$

Figure 2.10: Stability Contours for $(\gamma, c) = (0.25, 0.75)$
particular problem.

We begin by choosing a method (2.16) having fixed but arbitrary \( \gamma \) and \( c \). For the problem \( \dot{u} = au_x + \nu u_{xx}, \ a > 0 \), we apply this discretization scheme using spatial step size \( h \) and temporal step size \( k \). Let the time step restriction on \( k \) be \( \hat{k} \). Similarly, for the problem \( \dot{v} = a'v_x + \nu'v_{xx}, \ a' > 0 \) define \( h', k' \) and \( \hat{k}' \). Suppose \( \frac{\nu'}{a'h'} = \frac{\nu}{ah} \). Then the scaled (2.13) gives

\[
(\alpha'_j, \beta'_j) = \frac{a'/h'}{a/h} \left( \frac{2\nu}{h^2} \left( \cos(2\pi j h') - 1 \right), \frac{a}{h} \sin(2\pi j h') \right)
\]

which implies that the ellipse of Figure 2.1 is scaled by a factor \( \frac{a'/h'}{a/h} \). Setting \( k' = \frac{a/h}{a'/h'} k \) causes a similar scaling in the stability contours. Thus \( \frac{k'a'}{h'} = \frac{ka}{h} \), and so it is consistent to plot \( \frac{ka}{h} \) as a function of \( \frac{\nu}{ah} \).

The quantity \( \frac{\nu}{ah} \) represents the ratio of viscous effects to convective effects between mesh points. The inverse quantity

\[
R = \frac{ah}{\nu}
\]

has been referred to as the mesh Reynolds number (see Peyret and Taylor[17]).

As can be seen from Figures 2.11 to 2.13, increasing \( \gamma \) allows larger stable time steps when \( \frac{\nu}{ah} > \frac{1}{2} \). The case \( c = 1 - \gamma \) also has the property that decreasing \( \gamma \) allows larger time steps for \( \frac{\nu}{ah} < \frac{1}{2} \). Comparison of Figures 2.11 to 2.13 indicates that the largest time step can be applied using SBDF for \( \frac{\nu}{ah} > \frac{1}{2} \) and CNLF for \( \frac{\nu}{ah} < \frac{1}{2} \). This result physically corresponds to selecting SBDF when discrete diffusion dominates, and CNLF when discrete convection dominates. From this perspective, the popular CNAB is only competitive when \( \frac{\nu}{ah} \approx \frac{1}{2} \).

Frequently, an important consideration when choosing a second order scheme is what the constant of the truncation error is. For example, Crank-Nicolson is known to have a much smaller truncation error than second order BDF (see Hairer et al.[11]), so we expect CNAB to have a smaller truncation error than SBDF. Modified CNAB is expected to
Figure 2.11: Time Step Restriction For Various $\gamma$ where $c = 1 - \gamma$

have a truncation error similar to CNAB, however. (Numerical experiments in Chapter 4 support this claim.) Because of its small truncation error and because it produces stronger high frequency spatial decay than CNAB, modified CNAB may be preferred in certain problems over CNAB or SBDF when $\frac{\nu}{ah} > \frac{1}{2}$. To obtain a better understanding of the relative efficiencies of second order IMEX schemes, a study of the truncation errors would be useful.

Although the results of this section can be applied to a wide variety of problems, we still seek a method which is stable for all $\nu \geq 0$ and has strong decay for $|\alpha| \gg 1/k$. To achieve these objectives the next chapter examines higher order IMEX schemes.
Figure 2.12: Time Step Restriction For Various $\gamma$ where $c = \frac{(1-\gamma)^2}{2}$.

Figure 2.13: Time Step Restriction For Various $\gamma$ where $c = 0$. 
Chapter 3

Higher Order IMEX Schemes

None of the second order IMEX schemes have all the stability characteristics we desire. CNLF is stable for all \( \nu \leq 0 \) in the linear case, but has poor decay for large \(|\alpha|\). SBDF has good stability characteristics for \( \alpha \ll -1/k \) but has a very strict time step restriction for small \(|\alpha|\). Furthermore, no two-step, second order method contains the \( \beta \)-axis within its stability region.

To find a scheme satisfying all the desired stability properties we now consider higher order IMEX methods.

3.1 Third Order IMEX Schemes

We begin by deriving third order, 3-step IMEX schemes for \( \dot{u} = f(u) + \nu g(u) \). From Section 2.2, these schemes form a three parameter family of methods. One possible parameterization yields,

\[
\frac{1}{k} \left[ \left( \frac{1}{2} \gamma^2 + \gamma + \frac{1}{3} + \theta \right) u^{n+1} + \left( -\frac{3}{2} \gamma^2 - 2\gamma + \frac{1}{2} - \theta \right) u^n + \right. \\
\left. \left( \frac{3}{2} \gamma^2 + \gamma - 1 \right) u^{n-1} + \left( -\frac{1}{2} \gamma^2 + \frac{1}{6} \right) u^{n-2} \right] = \\
\left( \frac{\gamma^2 + 3\gamma}{2} + 1 + \frac{23}{12} \theta \right) f(u^n) - (\gamma^2 + 2\gamma + \frac{4}{3} \theta) f(u^{n-1}) + \left( \frac{\gamma^2 + \gamma}{2} + \frac{5}{12} \theta \right) f(u^{n-2}) + \\
\nu \left[ (\frac{\gamma^2 + \gamma}{2} + c) g(u^{n+1}) + (1 - \gamma^2 - 3c + \frac{23}{12} \theta) g(u^n) + \\
(\frac{\gamma^2 - \gamma}{2} + 3c - \frac{4}{3} \theta) g(u^{n-1}) + \left( \frac{5}{12} \theta - c \right) g(u^{n-2}) \right].
\]

(3.25)
These schemes are centred about time step \((n + \gamma)\) to third order, provided \(\theta = 0\). As for lower order schemes, the value of \(\gamma\) should be between 0 and 1 to avoid large truncation error. Also, the parameter \(c\) is multiplied by \(\nu\), so this parameter should be adjusted to modify large \(\nu\) properties of a scheme.

Some of these methods are familiar. Letting \(\theta \to \pm \infty\) yields

\[
\frac{1}{k}(u^{n+1} - u^n) = \frac{23}{12}[f(u^n) + g(u^n)] - \frac{4}{3}[f(u^{n-1}) + g(u^{n-1})] + \frac{5}{12}[f(u^{n-2}) + g(u^{n-2})]
\]

which is the third order Adams-Bashforth method.

Setting \((\gamma, \theta, c) = (1, 0, 0)\) yields

\[
\frac{1}{k}\left(\frac{11}{6}u^{n+1} - 3u^n + \frac{3}{2}u^{n-1} - \frac{1}{3}u^{n-2}\right) = 3f(u^n) - 3f(u^{n-1}) + f(u^{n-2}) + \nu g(u^{n+1})
\]

which is the third order BDF for the implicit part, and similarly to Section 2.5 is called third order SBDF.

Having determined integration formulae, we direct our attention to obtaining stability properties for third order IMEX schemes.

### 3.2 Choice of parameters

The third degree characteristic polynomial resulting from Equation (3.25) applied to \(\dot{z} = (\alpha + i\beta)z\) is given by

\[
\Phi(z) = \left[\frac{1}{2}\gamma^2 + \gamma + \frac{1}{3} + \theta - \left(\frac{\gamma^2 + \gamma}{2} + c\right)\alpha k\right]z^3
\]

\[-\left[\frac{3}{2}\gamma^2 + 2\gamma - \frac{1}{2} + \theta - \left(\frac{\gamma^2 + 3\gamma}{2} + 1 + \frac{23}{12}\theta\right)i\beta k + (1 - \gamma^2 - 3c + \frac{23}{12}\theta)\alpha k\right]z^2
\]

\[+ \left[\frac{3}{2}\gamma^2 + \gamma - 1 + (\gamma^2 + 2\gamma + \frac{4}{3}\theta)i\beta k + (\frac{\gamma - \gamma^2}{2} - 3c + \frac{4}{3}\theta)\alpha k\right]z
\]

\[-\left[\frac{1}{2}\gamma^2 - \frac{1}{6} + \left(\frac{\gamma^2 + \gamma}{2} + \frac{5}{12}\theta\right)i\beta k + (\frac{5}{12}\theta - c)\alpha k\right].
\]  

(3.27)

We now determine which methods produce the strongest asymptotic decay as \(\alpha \to -\infty\).

For this case, the roots of the characteristic polynomial (3.27) are given approximately
by
\[
\left(\frac{\gamma^2 + \gamma}{2} + c\right)z^3 + (1 - \gamma^2 - 3c + \frac{23}{12} \theta)z^2 - \left(\frac{\gamma - \gamma^2}{2} - 3c + \frac{4}{3} \theta\right)z + \frac{5}{12} \theta - c = 0. \tag{3.28}
\]
By determining the solutions, \(\tau_1, \tau_2\) and \(\tau_3\), of Equation (3.28) we may evaluate
\[
D_{\gamma, \theta, c} \equiv \max(|\tau_1|, |\tau_2|, |\tau_3|)
\]
to obtain an estimate of the high frequency model decay for large \(\nu\). Minimization over \((\gamma, \theta, c)\) determines the method with the strongest asymptotic high frequency decay. Certainly if
\[
D_{\gamma_0, \theta_0, c_0} = 0 \tag{3.29}
\]
then \((\gamma_0, \theta_0, c_0)\) minimizes the amplification as \(\alpha \to -\infty\). From Equation (3.28) we satisfy (3.29) iff
\[
\begin{align*}
1 - \gamma_0^2 - 3c_0 + \frac{23}{12} \theta_0 &= 0 \\
2\gamma_0^2 - \gamma_0^4 + 3c_0 - \frac{4}{3} \theta_0 &= 0 \\
\frac{5}{12} \theta_0 - c_0 &= 0.
\end{align*} \tag{3.30}
\]
Each term is divided by \((\gamma_0^2 + c_0)\) to allow the possibility of satisfying Equation (3.29) by letting \((\gamma_0^2 + c_0) \to \pm \infty\). Simplification of the system (3.30) yields
\[
\begin{align*}
\left(3\gamma_0 - 1\right)(\gamma_0 - 1) &= 0 \tag{3.31} \\
\theta_0 - 6(\gamma_0^2 - \gamma_0) &= 0 \tag{3.32} \\
\frac{5}{12} \theta_0 - c_0 &= 0. \tag{3.33}
\end{align*}
\]
For \((\frac{\gamma^2 + \gamma_0}{2} + c_0)\) finite there are two possibilities, \((\gamma_0, \theta_0, c_0) = (1, 0, 0)\) and \((\gamma_0, \theta_0, c_0) = (\frac{1}{3}, -\frac{4}{3}, -\frac{5}{3})\), both of which specify third order SBDF. For \((\frac{\gamma^2 + \gamma_0}{2} + c_0)\) infinite, Equation (3.31) implies \(\gamma_0 \ll |c_0|\). Using this in Equation (3.32) implies \(|\theta_0| \ll |c_0|\). Applying these results to Equation (3.33) results in a contradiction, so \((\frac{\gamma^2 + \gamma_0}{2} + c_0)\) must be finite.

Because third order SBDF has the strongest asymptotic decay of third order IMEX schemes, special attention is given to its properties throughout the remainder of this chapter.

### 3.3 Third Order Stability along the \(\beta\)-Axis

We begin by verifying stability at the origin \((\alpha, \beta) = (0, 0)\). From Equation (3.27) the roots of the characteristic equation at the origin are given by

\[
(\tau - 1)[(\frac{1}{2} \gamma^2 + \gamma + \frac{1}{3} + \theta)\tau^2 + (\gamma^2 + \gamma - \frac{5}{6})\tau + \frac{1}{2} \gamma^2 - \frac{1}{6}] = 0
\]

To be stable all roots must have magnitude less than or equal to 1, and those having absolute value 1 must be simple. Third order SBDF, as well as the methods of Section 3.4 satisfy this criteria.

Stability along the \(\beta\)-axis is verified by considering the application of third order methods to the one-dimensional wave equation. We demonstrate this technique for third order SBDF. Applying Equation (3.26) to \(\dot{x} = i\beta x\) we obtain the characteristic polynomial

\[
\varphi_0(z) = \frac{11}{6}z^3 - 3(1 + i\beta k)z^2 + (\frac{3}{2} + 3i\beta k)z - \frac{1}{3} - i\beta k
\]

Using the definitions of Section 2.4 we determine that

\[
|\varphi_0^*(0)|^2 = 3.3611 > .1111 + 1.0000\beta^2 = |\varphi_0(0)|^2
\]

for \(|\beta|\) sufficiently small. Using the symbolic computation package Maple[7] we find that \(\varphi_1(z) \neq 0\) and that

\[
|\varphi_1^*(0)|^2 = 10.5625 - 6.5000\beta^2 + 1.0000\beta^4 > 3.0625 + 1.7450\beta^2 + 9.0000\beta^4 = |\varphi_1(0)|^2
\]
for $|\beta|$ sufficiently small. Reapplying Definition 2.4.4 we determine that the square of the absolute value of the root of $\varphi_2(z)$ is given by

$$\frac{56.25 - 123.75\beta^2}{56.25 - 123.75\beta^2 - 88.50\beta^4 + 234.25\beta^6 + 36.00\beta^8}$$

which is less than 1 on the nonzero $\beta$-axis near the origin. Thus $\varphi_0(z)$ is a von Neumann polynomial by repeated application of Theorem 2.4.1, and so Theorem 2.4.2 assures us that third order SBDF is stable on the $\beta$-axis for $\beta$ sufficiently small.

Similar studies for the methods described in the next section indicate that they also include the $\beta$-axis in the absolute stability region.

### 3.4 Third Order Stability Contours

Further information about stability in the $\alpha$-$\beta$ plane can be obtained by plotting $\max\{|z|: \Phi(z) = 0\}$, where $\Phi(z)$ is defined in Equation (3.27). These stability contours are displayed in Figures 3.14 to 3.19.

We begin by examining if it is possible to arrive at a stable scheme for any fixed $\gamma$. For a fixed, but arbitrary $\gamma$ and for $|\theta|, |c| \to \infty$ we obtain an approximate local minimum of $D_{\alpha,\theta,c}$ if $\frac{\varepsilon}{\delta} = 0.4661$. Using these parameters, the scheme simplifies to

$$\frac{1}{k}(u^{n+1} - u^n) = \frac{23}{12} f(u^n) - \frac{4}{3} f(u^{n-1}) + \frac{5}{12} f(u^{n-2}) + .4661\nu g(u^{n+1}) + .5184\nu g(u^n) + .0650\nu g(u^{n-1}) - .0494\nu g(u^{n-2})$$

(3.35)

which applies third order Adams-Bashforth to the explicit term. The stability contours of Figure 3.14 suggest that this method is stable for all $\nu \geq 0$ provided $k < 0.62\frac{\nu}{\delta}$. This restriction is more severe than that for third order Adams-Bashforth applied to $\dot{x} = i\beta x$ because of the dip in the stability contours when $\alpha < 0$. Careful analysis similar to that of the previous section verifies that the $\beta$-axis is included in the absolute stability region.
This result demonstrates that for third order methods, it is possible to find methods for any $\gamma$ which are stable for all $\nu \geq 0$ by varying $\theta$ and $c$.

In Chapter 2, the most interesting second order schemes were produced by selecting $\gamma$ equal to $0, \frac{1}{2}$ or 1. We consider schemes for these values of $\gamma$ below. The parameters $\theta$ and $c$ are chosen to produce schemes which allow large stable time steps as $\nu \to \infty$.

For example, the method $(\gamma, \theta, c) = (0, -2.036, -0.876)$ of Figure 3.15 is stable for all $\nu \geq 0$ provided $k \leq 0.67 \frac{h}{a}$. Similarly $(\gamma, \theta, c) = (.5, -1.21, -0.5)$ of Figure 3.17 is stable for all $\nu \geq 0$ if $k \leq 0.65 \frac{h}{a}$. In both these cases substantially larger time steps can be taken for large or moderate $|\alpha|$ than for the method (3.35). Furthermore, stronger high frequency decay occurs for these methods than for method (3.35).

From Section 3.2 we know that the strongest decay as $\alpha \to -\infty$ occurs for third order SBDF. The stability contours for this method are shown in Figure 3.18. This plot together with the zoom-in of Figure 3.19 suggest that third order SBDF is stable for all $\alpha \leq 0$ provided $k < 0.62 \frac{h}{a}$. The plot of Figure 3.18 also indicates that very large time steps can be taken for large or moderate $|\alpha|$. Although applying $\gamma = 1$ and nonzero $\theta$ and $c$ may allow somewhat larger stable time steps we focus on $\theta = c = 0$ since other choices degrade the strong asymptotic decay.

For $\gamma \neq 1$, the choice $\theta = c = 0$ is not recommended. As seen in Figure 3.16, $(\gamma, \theta, c) = (\frac{1}{2}, 0, 0)$ results in a small stability region. This plot indicates that very small time steps are needed for moderate or large $\frac{\nu}{h^2}$, since the ellipse of Figure 2.1 must lie in the stable region.
Figure 3.14: Stability Contours for $(\gamma, \theta, c) = \lim_{\theta \to \infty} (\gamma, \theta, .4661\theta)$

Figure 3.15: Stability Contours for $(\gamma, \theta, c) = (0, -2.036, -.876)$
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Figure 3.16: Stability Contours for \((\gamma, \theta, c) = \left(\frac{1}{2}, 0, 0\right)\)

Figure 3.17: Stability Contours for \((\gamma, \theta, c) = \left(\frac{1}{2}, -1.21, -.5\right)\)
Figure 3.18: Stability Contours for Third Order SBDF, \((\gamma, \theta, c) = (1, 0, 0)\)

Figure 3.19: Zoom-in Around \(\alpha = 0\) for Third Order SBDF
3.5 Fourth Order IMEX Schemes

From Section 2.2, the general fourth order, four-step IMEX scheme is a four parameter family of methods. From the previous section we anticipate that the fourth order semi-implicit backwards differencing formula (fourth order SBDF) may have good stability properties. For \( \dot{u} = f(u) + \nu g(u) \), this scheme is given by

\[
\frac{1}{k} \left( \frac{25}{12} u^{n+1} - 4u^n + 3u^{n-1} - \frac{4}{3} u^{n-2} + \frac{1}{4} u^{n-3} \right) = 4f(u^n) - 6f(u^{n-1}) + 4f(u^{n-2}) - f(u^{n-3}) + \nu g(u^{n+1}).
\]  

(3.36)

The characteristic polynomial obtained from applying Equation (3.36) to \( \dot{x} = (\alpha + i\beta)x \) is

\[
\Phi(z) = \left( \frac{25}{12} - \alpha k \right) z^4 - (4 + 4i\beta k) z^3 + (3 + 6i\beta k) z^2 - \left( \frac{4}{3} + 4i\beta k \right) z + \frac{1}{4} + i\beta k.
\]

Clearly, all of the characteristic roots tend to 0 as \( \alpha \to -\infty \) so the amplification must tend to 0 as \( \alpha \to -\infty \). Similar to the proof of Section 3.3, repeated application of Theorem 2.41 using Maple[7] shows that the \( \beta \)-axis is included in the stability region. Furthermore, the characteristic stability contours plotted in Figure 3.20 indicate that fourth order SBDF is stable for \( k \leq 0.52 \frac{h}{a} \) and that larger time steps are permitted as \( \nu \) increases.

Comparison of Figures 3.18 and 3.20, however, indicates that the stability region is smaller than for the third order case, so smaller time steps may be required. Furthermore, comparison of Figures 3.19 and 3.21 shows that the \( \beta \)-axis is closer to the boundary of the stability region for fourth order SBDF, suggesting that third order SBDF may dissipate error better for \( \nu \approx 0 \).
Figure 3.20: Stability Contours for Fourth Order SBDF

Figure 3.21: Zoom-in Around $\alpha = 0$ for Fourth Order SBDF
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3.6 Comparison to Lower Order Methods

Third and fourth order SBDF methods are good choices for IMEX schemes for some problems. For all \( \nu \geq 0 \), these methods are stable for a time step restriction similar to the CFL condition. Greater accuracy and strong high frequency decay also make these methods very attractive. Nonetheless, for many problems second order methods are preferred. Higher order methods require more storage, and more work per time step. This extra expense could be justified if greater accuracy permitted larger time steps. Third and fourth order schemes, however, have more severe time step restrictions than second order schemes. In fact, Figure 3.22, shows that larger stable time steps can be taken with second order SBDF when \( \frac{\nu}{a h} > .11 \) for the linear advection-diffusion problem using second order spatial discretizations. CNLF allows larger stable time steps than either third or fourth order SBDF for \( \frac{\nu}{a h} < 1 \).

Third order SBDF should be efficient for problems which require strong decay for \( |\alpha| \gg 1/k \) and a moderate time step restriction for \( \frac{\nu}{a h} < 0.1 \). It should also be effective for problems where \( \frac{\nu}{a h} \ll 1 \), since the \( \beta \)-axis is within the stability region.

Fourth order SBDF has a particularly severe time step restriction for the advection-diffusion problem when \( \frac{\nu}{a h} \) is moderate or large. For example, when \( \frac{\nu}{a h} = 8 \), fourth order SBDF only can apply one tenth the time step of second order SBDF, as can be seen from Figure 3.22. This restriction on the step size would appear to limit fourth order SBDF to problems where accuracy, and not stability is the reason for limiting the time step size.
Figure 3.22: Time Step Restrictions for Various IMEX Schemes
Chapter 4

Convection-Diffusion Experiments

The previous chapters have dealt with stability properties of IMEX schemes for the one-dimensional linear constant coefficient advection-diffusion equation. These results provide necessary, but not sufficient conditions for stability for variable coefficient and nonlinear convection-diffusion problems.

The next sections summarize numerical experiments which verify our analysis for the simple, linear problem can be useful for determining which IMEX scheme to apply to more complicated problems. In particular, strongly damping schemes are shown to be more efficient in certain spectral collocation and multigrid applications. In order to calculate starting values for multistep IMEX schemes, we use one-step (low order) IMEX schemes with a very small time step, unless otherwise noted.

4.1 Finite Difference Approximations

4.1.1 Variable Coefficient Problem

To examine nonzero viscosity behaviour, we consider the one-dimensional variable coefficient problem

\[ u_t + \sin(2\pi x)u_x = \nu u_{xx} \quad (4.37) \]

subject to periodic boundary conditions on the interval [0,1] and initial condition

\[ u(x,0) = \sin(2\pi x). \]
Because shocks or other discontinuities do not form for any \( \nu \geq 0 \) for this problem, we expect that centred differences can be used to compute accurate approximate solutions for this example provided a sufficiently fine spatial mesh is applied. For this reason, the next two sections use second order centred differences \( D_1 \) and \( D_2 \), as defined in Section 2.3, to approximate \( u_x \) and \( u_{xx} \).

### 4.1.2 Small Mesh Reynolds Number Computations

To test the theory's predictions for small mesh Reynolds numbers (2.24), the model problem (4.37) was approximately solved using discretization step sizes \( h = \frac{1}{63} \) in space and \( k = 1.8h \) in time. Use of such step sizes is appropriate only for strongly damped flow. Utilizing several IMEX schemes, computations to time \( t = 2 \) are performed for viscosities, \( \nu \), in the range \( .01 \leq \nu \leq .1 \). These values correspond to mesh Reynolds numbers, \( R \), in the range \( 1.59 \geq R \geq 0.159 \).

From Figures 2.11, 2.12, 2.13 and 3.22 the theory predicts that for these step sizes SBDF is stable for a larger viscosity interval than any other scheme. As \( \nu \) decreases, third order SBDF followed by CNAB should become unstable. Stability for modified CNAB should be similar to, and somewhat better than, CNAB. Furthermore, fourth order SBDF and CNLF should be unstable over the entire interval because the theoretical stability restriction is violated.

By comparing results to those for \( h = \frac{1}{504} \) and \( k = .225h \) using SBDF, the max norm relative errors for second order schemes are evaluated. Third and fourth order schemes are compared to computations with these same step sizes but using third and fourth order SBDF. The resultant errors are plotted against \( \nu \) in Figure 4.23. Fourth order SBDF and CNLF are not included because they are unstable over the entire interval. The plots of the figure clearly coincide with the results of the theory.

Figure 4.23 also indicates that SBDF is the only stable method for the above choice
of discretization parameters when $0.0015 < \nu < 0.0025$. This agrees with the prediction that SBDF allows the largest stable time steps for small mesh Reynolds numbers (see Section 2.11). Although third order SBDF has a smaller stability interval, it may be useful in problems where high accuracy is needed since it produces a smaller error than second order methods when stable.

For the second order family of schemes (2.16) such that $\gamma = \frac{1}{4}$, plots for several $c$ are made. These are displayed in Figure 4.24. Although the best asymptotic decay occurs for $c = .28125$ (see Section 2.7), a wider variety of viscosities can be computed with other choices of $c$. An interesting and open problem would be to determine which second order scheme for a given $\gamma$ permits the largest stable time steps when $\nu \gg 1/k$. The choice $c = 1 - \gamma$ appears to allow particularly large time steps for $\nu \gg 1/k$.

To conclude, Example (4.37) supports several of the theoretical results for small mesh Reynolds numbers. In particular, SBDF seems to be a good choice when the largest stable steps are desired and third order SBDF appears appropriate when higher accuracy is needed. Results for the large mesh Reynolds number case are considered next.

4.1.3 Large Mesh Reynolds Number Computations

To test the theory's predictions for large mesh Reynolds numbers, example (4.37) was solved using discretization step sizes $h = \frac{1}{81}$ in space and $k = .9h$ in time. Using several IMEX schemes, computations to time $t = 2$ are performed for viscosities, $\nu$, in the range $.001 \leq \nu \leq .01$. These values correspond to mesh Reynolds numbers, $R$, in the range $12.3 \geq R \geq 1.23$.

From Figures 2.11, 2.12, 2.13 and 3.22 the theory predicts that for these step sizes only CNLF is stable over the entire viscosity interval. As $\nu$ decreases, third order SBDF followed by SBDF and finally CNAB should become unstable. Stability for modified CNAB should be similar to CNAB. Furthermore, fourth order SBDF should be unstable
Figure 4.23: Large Viscosity Behaviour For Various IMEX Methods

Figure 4.24: Second Order Results for $\gamma = \frac{1}{4}$ for Various $c$
over the entire interval because the theoretical stability restriction is violated when \( \nu < .05 \) for these step sizes.

By comparing results to those for \( h = \frac{1}{648} \) and \( k = .225h \) using SBDF, the max norm relative errors for second order schemes are evaluated for these computations. Third and fourth order schemes are compared to computations with these same step sizes but using third and fourth order SBDF. The resultant errors are plotted against \( \nu \) in Figure 4.25. Fourth order SBDF is not plotted because it is unstable over the entire interval. The plots of the figure support the results of the theory.

Figure 4.25 also indicates that CNLF is the only stable method for \( \nu < 0.002 \). This agrees with the prediction that CNLF allows the largest stable time steps for large mesh Reynolds numbers (see Section 2.11). CNLF is a particularly attractive choice because it has the smallest error of second order methods. Use of SBDF is not recommended because it has the smallest stable interval and the largest error of any second order scheme.

For the same problem using \( k = .5h \), dramatically different results are predicted because all the methods satisfy their theoretical stability restrictions. Indeed, computations for CNLF, third and fourth order SBDF all produce errors which nearly coincide, since spatial error dominates the solutions. Other second order methods appear stable and produce only slightly less accurate results.

To obtain more information about the behaviour of the solution for \( \nu \) near 0, we next examine a problem for which \( \nu = 0 \).

### 4.1.4 Zero Viscosity Computations

To examine the limit \( \nu = 0 \), we consider the one-dimensional nonlinear problem

\[
\frac{u_t}{2} + \cos(2\pi t)(1 + u)u_x = 0
\]  

(4.38)
having periodic boundary conditions on the interval \([0,1]\) and initial conditions

\[ u(x,0) = \sin(2\pi x). \]

As in the previous two sections, we use second order centred differences to approximate \(u_x\) and \(u_{xx}\). For \(h = \frac{1}{80}\) and \(k = .5h\), computations are performed to time \(t = 100\). The time step value \(k = .5h\) was used to ensure that fourth order SBDF satisfied the stability restriction \(k \leq .52h\). Using the fact that the exact solution to this problem at integer \(t\) equals the initial data, i.e.

\[ u(x,n) = \sin(2\pi x), \; n = 0,1,2,\ldots \]

we compute the error in the solution at time \(t = n, n = 1,2,\ldots, 100\). The relative max norm errors for several schemes are plotted in Figures 4.26 and 4.27.

All second order schemes tested, such that \(\gamma > 0\), were unstable. This result supports the conclusion of Section 2.8. CNLF, third order SBDF and fourth order SBDF were all stable.
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The error at \( t = 100 \) for CNLF was less than \( 10^{-7} \). This method performs extremely well for this example since it is a time reversible method. It is known that leap frog is only stable for \( \nu = 0 \), however. Thus CNLF may be more sensitive to perturbations of the eigenvalues away from the \( \beta \)-axis than third or fourth order SBDF.

As can be seen in Figure 4.27, the error for third order SBDF is concave down as \( t \) increases and has a final value of 4% at \( t = 100 \). The fact that the error is concave down supports the conclusion that the \( \beta \)-axis is included in the stable region, since error is being dissipated.

For fourth order SBDF, the theory predicts that the \( \beta \)-axis is stable, but that it is much closer to the boundary of the stability region. Examination of the error to four significant digits verifies that dissipation occurs for fourth order SBDF. Because the dissipation is very weak, the growth of the error appears linear as can be seen in Figure 4.27.

In summary, CNLF, third and fourth order SBDF perform well for the zero viscosity case. Of these schemes, CNLF is non-dissipative while third order SBDF is the most strongly dissipative. To obtain more information about the zero viscosity case, a linear analysis of the phase lag error would be a useful undertaking.

The next few sections consider problems with a stronger physical motivation.

4.2 Spectral Collocation

4.2.1 The Burgers Equation

For our next application we consider the Burgers equation,

\[
    u_t + uu_x = \nu u_{xx}
\]  

(4.39)
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Figure 4.26: Zero Viscosity Example For Various Second Order Methods, $\gamma$

Figure 4.27: Zero Viscosity Example For Higher Order Methods
subject to periodic boundary conditions on the interval $[-1,1]$ and initial conditions

$$u(x,0) = \sin(\pi x).$$

We expect that spectral solutions for this equation provide information about numerical solutions to more complicated problems such as the Navier-Stokes equations.

A plot of the solution of the Burgers equation for $\nu = .01$ at several different times is provided in Figure 4.28. This computation was produced using Chebyshev collocation with 40 basis functions and $k = 1/160$ using SBDF.

The next few sections discuss Fourier and Chebyshev collocation implementations for the above model problem. See Canuto et al.[6] or Boyd[2] for details on these methods.
4.2.2 Fourier Spectral Collocation

Since the problem of this section is periodic, we expect that Fourier series makes a good basis of trial functions for this problem. Indeed, since

\[ u_t = -\frac{1}{2} \frac{\partial u}{\partial x} + \nu \frac{\partial^2 u}{\partial x^2} \]

we see that \( u_t \) is antisymmetric for \( u \) antisymmetric. By selecting an initial condition which is antisymmetric we guarantee that \( u \) remains antisymmetric for all \( t \). Since only these components of the series contribute to the solution we use a Fourier sine series. We thus approximate \( u \) by the series

\[ u_N(x, t) = \sum_{j=1}^{N} \alpha_j(t) \sin(jx). \]

To determine \( \alpha_j(t) \), we enforce the differential equation at the collocation points,

\[ \left[ \frac{\partial u_N}{\partial t} + u_N \frac{\partial u_N}{\partial x} = \nu \frac{\partial^2 u_N}{\partial x^2} \right]_{x=x_j}, \]

where \( \alpha_1(0) = 1 \) and \( \alpha_j(0) = 0, j \neq 1 \). This scheme is also called a pseudospectral method since the nonlinear convection term is evaluated in physical space.

By applying Fourier sine collocation with 40 basis functions and \( k = 1/40 \), we solve the model problem at each time step to time \( t = 2 \). Because the system is small, the implicit equations are solved in physical space using LU decomposition. In larger systems where greater efficiency is needed these would be solved in Fourier space using transform methods (see Canuto et al.[6]). For CNAB, modified CNAB, SBDF and third order SBDF the max norm relative error is plotted against viscosity (see Figure 4.29). For second order schemes, the “exact solution” is based on a computation using \( N = 80 \) modes and \( k = \frac{1}{3200} \) using SBDF. A computation using \( N = 80, k = \frac{1}{3200} \) and third order SBDF provides the “exact solution” in the third order case.
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Figure 4.29: Fourier Spectral Collocation for Burgers Equation

CNLF was not included because the theoretical stability restriction is violated. This can be easily seen because the linear advection-diffusion equation has eigenvalues \((iαnπ − νn^2π^2)\) for eigenfunctions \(e^{inπx}\). From these eigenvalues we know that the stability restriction is \(k < \frac{1}{αn}\), which is violated initially because \(|u(x, 0)|_∞ = 1\).

As expected, third order SBDF has the smallest error of any of the methods when stable. The stable region, however, is smaller than that for CNAB or SBDF. CNAB and modified CNAB are once again very similar in behaviour with the modified version being marginally better. SBDF appears to allow the largest stable time step when \(ν ≈ 0.01\).

Further refinement of the time step to \(k = \frac{1}{160}\) leaves third order SBDF as the method of choice over the entire interval. Such a refinement seems unnecessary in this example because the error is less than 1% for a step size which is 4 times larger.
4.2.3 Chebyshev Spectral Collocation

Because the solution to the problem is periodic and anti-symmetric we know that \( u(\pm 1, t) = 0 \) for all \( t \). Using this fact, we solve (4.39) subject to the homogeneous Dirichlet boundary conditions \( u(\pm 1, t) = 0 \), using a pseudospectral Chebyshev collocation scheme. The Gauss-Chebyshev grid,

\[
x_i = \cos[(2i - 1)\pi/2N], \quad i = 1, \ldots, N
\]

is used for collocation points.

Similar to the Fourier case, the max norm relative errors are evaluated for several IMEX schemes using \( k = 1/40 \) and \( N = 40 \). As can be seen from Figure 4.30, the results are qualitatively similar to those of the Fourier case. SBDF performs particularly well for smaller viscosities. From the theory, it has the widest stability region for large \( |\alpha| \) and thus is best able to accommodate the rapidly growing eigenvalues associated with Chebyshev collocation.

Both Chebyshev and Fourier collocation can be affected by aliasing (see Canuto et al.[6]). We consider aliasing for the Fourier case next.

4.2.4 Aliasing in Pseudospectral Methods

Aliasing occurs when nonlinear terms produce frequencies that cannot be represented in the basis, and thus contribute erroneously to lower frequencies.

For example, in the Burgers equation, the Fourier sine mode \( \sin(mx) \), when explicitly evaluated in the convection term produces the contribution \( \sin(mx) \frac{\partial \sin(mx)}{\partial x} = m \sin(2mx) \). If \( 2m \) is greater than the number of Fourier sine basis functions, \( N \), this frequency cannot be represented correctly and aliasing occurs. We now proceed to demonstrate that this behaviour can plague poorly spatially resolved computations when applying weakly damping IMEX schemes.
We compute solutions for the model Burgers equation (4.39) subject to periodic boundary conditions and the initial conditions

\[ u(x,0) = 0.98 \sin(2\pi x) + HF(x) \]

where

\[ HF(x) \equiv 0.01 \sin(61\pi x) + 0.01 \sin(62\pi x). \]

We use Fourier sine collocation as described in Section 4.2.1 with \( N = 64 \) basis functions, and integrate to time \( t = 2 \).

The value of the approximate solution at time \( t = k \) is obtained using first order SBDF with the same step size. To represent the type of high frequency information that could be produced during a computation, we add \( HF(x) \) to the solution at \( t = k \). This ensures that high frequency information remains after the strongly damping first order SBDF step. Subsequent steps are then computed using the relevant second order
scheme. For third order SBDF, the value at $t = 2k$ is also needed. For the purpose of demonstrating aliasing effects, this value is computed using CNAB since we wish to retain most of the added high frequencies.

The max norm relative errors for several IMEX schemes are computed by comparing results to those for SBDF using $N = 128$ and $k = \frac{1}{24N}$. In the third order case, results are compared to those for third order SBDF using $N = 128$ and $k = \frac{1}{24N}$. These errors are summarized below.

<table>
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<th>$k$</th>
<th>CNLF</th>
<th>CNAB</th>
<th>Modified CNAB</th>
<th>SBDF</th>
<th>$3^{rd}$ order SBDF</th>
</tr>
</thead>
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<tr>
<td>$\frac{1}{64}$</td>
<td>.92</td>
<td>.575</td>
<td>.0056</td>
<td>.0072</td>
<td>.0045</td>
</tr>
<tr>
<td>$\frac{1}{192}$</td>
<td>.060</td>
<td>.022</td>
<td>.0013</td>
<td>.00079</td>
<td>.0010</td>
</tr>
</tbody>
</table>

For the case $k = \frac{1}{64}$, we note that the error for CNAB is far greater than for modified CNAB, SBDF or third order SBDF. Using CNAB, a non-aliased computation using the 2/3's rule as described in Section 1.3 and $k = \frac{1}{64}$ results in a relative error of less that $10^{-3}$. This non-aliased result, along with its aliased counterpart, are plotted in Figure 4.31. The "error" curve in this figure is that of the aliased CNAB. From the figure it is clear that the main component of the error is proportional to $\sin(\pi x)$. This low frequency mode is not part of the exact solution, and must be an aliasing artifact from high frequency components. It is interesting to note that even after 128 time steps the numerical solution is still plagued by high frequency components which have not yet decayed. A similar study of CNLF reveals that it suffers from aliasing as well.

Resorting to a smaller time step, $k = \frac{1}{192}$, makes a substantial improvement in the solution for CNAB and CNLF. Even so, the aliasing error for CNLF is sufficiently large that further refinement is likely required.

We conclude that use of a strongly damping scheme such as SBDF, modified CNAB
or third order SBDF gives an inexpensive method to reduce aliasing in poorly resolved computations. Application of weakly damping schemes like CNAB and especially CNLF may necessitate undesirably small time steps to produce the high frequency decay needed to prevent aliasing in an aliased computation. Alternatively, weakly damping schemes may be used in conjunction with an anti-aliasing technique such as the 3/2’s rule or the 2/3’s rule. However, as described in Section 1.3, these anti-aliasing techniques either increase the expense of the computation or produce a severe loss of high frequency information at each time step.

As we shall demonstrate in subsequent sections, strongly damping schemes can be desirable for solving the implicit equations in finite difference equations when using multi-grid.
4.3 Time-Dependent Multigrid

4.3.1 The Convection-Diffusion Problem

The next model that we consider is the 2D convection-diffusion problem,

\[ u_t + (\mathbf{u} \cdot \nabla)\mathbf{u} = \nu \Delta \mathbf{u} \quad (4.40) \]

where \( \mathbf{u} \equiv (u, v) \). This model incorporates some of the major ingredients of the 2D Navier-Stokes equations. Indeed, it is often being solved as part of projection schemes for incompressible flows (see Hirsch[12]). We carry out our computations on the square \( \Omega \equiv [0,1] \times [0,1] \) and consider periodic boundary conditions and initial conditions,

\[
    u(x, y, 0) = \sin[2\pi(x + y)] \\
    v(x, y, 0) = \sin[2\pi(x + y)].
\]

For spatial discretization we use standard centred differences. Thus we use \( \Delta_h \), the standard 5-point Laplacian, to approximate \( \Delta \) and

\[
    \nabla_h = \begin{pmatrix} D_x \\ D_y \end{pmatrix}
\]

where

\[
    D_x u_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2h} \\
    D_y u_{i,j} = \frac{u_{i,j+1} - u_{i,j-1}}{2h}
\]

to approximate \( \nabla \). For IMEX schemes the convection term, \( (\mathbf{u} \cdot \nabla)\mathbf{u} \), is handled explicitly and the diffusion term, \( \nu \Delta \mathbf{u} \), is handled implicitly.

This treatment yields a positive definite, symmetric, sparse linear system to solve at each time step. Such systems are solved efficiently using a multigrid algorithm, the components of which are outlined in the next section.
4.3.2 Components of the Multigrid Algorithm

To solve the implicit equations we apply a Full Multigrid (FMG), Full Approximation Scheme (FAS) algorithm (see Brandt[4]). Rather than applying the standard algorithm at each time step, we use the recent ideas of Brandt and Greenwald[5]. The main components of the resulting algorithm are outlined below.

Smoothing is accomplished using Red-Black Gauss-Seidel. This relaxation technique is chosen because it has a very good smoothing rate. Prolongation is accomplished using bilinear interpolation, and restriction by full weighting.

The standard FMG cycle is modified so that the first coarse grid correction is performed before any fine grid relaxation. Based on the assumption that the increment between time steps is smooth, Brandt and Greenwald[5] claim that fine grid relaxation is most effective after the smoothness of the increment is accounted for.

Interpolation for the FMG step is bilinear. Brandt and Greenwald[5] argue that for time-dependent problems higher order interpolation only decreases high frequency error, which tends to dissipate in parabolic systems anyway. This suggestion is utilized here, since experiments with cubic interpolation did not produce any reduction in the number of multigrid iterations to achieve a given tolerance.

Another recommendation of Brandt and Greenwald[5] is to avoid the final smoothing pass at each time step, in order to reduce aliasing from Red-Black Gauss-Seidel relaxation. Aliasing is not a major source of error in the model problem, so this suggestion does not improve accuracy or reduce the number of fine grid iterations. For these reasons, this suggestion was not utilized.

For this problem we use a residual test with a tolerance TOL to determine the number of fine grid iterations to perform at each time step. In the next section we show that the choice of time-stepping scheme can affect the number of fine grid iterations to achieve a
given residual tolerance.

### 4.3.3 Relative Efficiencies of Several IMEX Schemes

The model problem (4.40) was approximated using step sizes $h = \frac{1}{128}$ and $k = 0.00625$ and residual tolerance $\text{TOL}=0.003$. After the first time step, high frequency information

$$HF(x, y) = 0.005 \cos[2\pi(64x + 63y)]$$

was added to each of $u$ and $v$, to represent the type of high frequency information that might be produced during a computation.

For several second order IMEX schemes, the average number of fine grid iterations at each time step was computed. The result using V-cycles is graphed in Figure 4.32. Strongly damping schemes such as SBDF and modified CNAB require roughly 1 iteration per time step. Weakly damping schemes required far more effort to solve the implicit equations accurately, because lingering high frequency components necessitate more work on the finest grid. This is evident since CNAB requires more than 2 iterations per time step and CNLF required 3.

Using a W-cycle improves the relative efficiencies of CNLF and CNAB. Even for these cases, however, nearly twice the number of fine grid iterations were required than for more strongly damping schemes such as SBDF and modified CNAB. See Figure 4.33 for these results.

Even for a smaller viscosity, $\nu = 0.02$, and a much coarser mesh $h = \frac{1}{32}$, the performance of CNLF suffers. It uses about 30% more iterations than SBDF or modified CNAB to achieve the desired tolerance. This result uses $\text{TOL}=.009$ and is plotted in Figure 4.34.

Thus we conclude that use of a poorly damping IMEX scheme such as CNAB or especially CNLF can necessitate extra iterations on the finest grid in multigrid solutions.
to the implicit equations for small mesh Reynolds numbers, \( R < 2 \). For large mesh Reynolds, \( R > 2 \), this effect was not observed.

### 4.4 Choice of IMEX Scheme

Based on observations in this and previous chapters we provide a few guidelines for selecting IMEX schemes for convection-diffusion problems.

#### 4.4.1 Finite Differences

For the finite difference case, begin by determining an estimate for the inverse of the mesh Reynolds number, \( \frac{\nu}{ah} \), where \( \nu \) represents viscosity, \( a \) and \( h \) represent characteristic speed and grid spacing.

For problems where \( \frac{\nu}{ah} \ll \frac{1}{2} \) application of CNLF, or a third or fourth order scheme is reasonable. A study to determine the optimal higher order scheme for \( \frac{\nu}{ah} \ll \frac{1}{2} \) would
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Figure 4.33: Multigrid W-Cycle Iterations, $\nu = 0.03, h = \frac{1}{128}$

Figure 4.34: Multigrid W-Cycle Iterations, $\nu = 0.02, h = \frac{1}{32}$
be interesting. Third and fourth order SBDF, can be applied to these problems, since the $\beta$-axis is included in the stability region even though these methods were selected primarily for their large $\nu$ properties. Of the methods we have considered in detail, CNLF has the mildest time step restriction and is non-dissipative while third order SBDF is the most dissipative. All other second order schemes should be avoided in this case. Explicit schemes should also be considered for these problems.

For $0 < \frac{\nu}{a h} < \frac{1}{2}$ use of CNLF or third order SBDF appears appropriate. CNLF has the mildest time step restriction, but accuracy concerns could make third order SBDF competitive. Avoid use of SBDF in this case. For problems of this type, a study to determine when explicit schemes are competitive would be interesting.

For $\frac{\nu}{a h} \approx \frac{1}{2}$ the theory predicts that many second order IMEX schemes have similar time step restrictions. A study to determine the method with the smallest truncation error would be useful in this case. For greater accuracy, third order SBDF appears to be more useful than fourth order SBDF, since its time step restriction is less severe. If strong decay of high frequency spatial modes is a desirable characteristic modified CNAB can be used.

For $\frac{\nu}{a h} > \frac{1}{2}$, use of SBDF permits the largest stable time steps. Modified CNAB can also be applied to problems of this type, although its time step restriction is somewhat stricter. Third order SBDF is recommended when high accuracy is needed. Numerical experiments in Section 4.3 demonstrate that in multigrid solutions to the implicit equations, application of a strongly damping method is prudent. Modified CNAB or SBDF should be useful in such problems. Avoid use of CNLF in this case.

4.4.2 Spectral Methods

Because the eigenvalues for spectral methods are different than for finite differences as is their meaning (see Trefethen[20]), we cannot expect the stability time step restrictions
from Sections 2.7 and 3.6 to hold quantitatively. For this reason, an analysis of the linear advection-diffusion equation for Chebyshev and Fourier spectral methods would be interesting.

Numerical experiments for the Burgers equation were made for small to moderate mesh Reynolds numbers. For these problems, CNLF has a very severe time step restriction. These computations also suggest that SBDF has the mildest time step restriction of the methods considered. This result is particularly pronounced in the Chebyshev collocation case.

The large mesh Reynolds number case for spectral collocation was not considered. In this case, a comparison of the relative efficiencies of IMEX schemes and fully explicit schemes would be interesting.

Third order SBDF appears to be an efficient method for problems where high accuracy is needed.

In problems where aliasing occurs, a strongly damping scheme, such as SBDF, modified CNAB or third order SBDF can be used to inexpensively reduce aliasing. Application of a weakly damping scheme such as CNAB or CNLF in poorly spatially resolved, aliased computations should be avoided.
Chapter 5

Reaction-Diffusion Experiments

The previous chapters focus on the application of IMEX schemes to convection-diffusion problems. We now examine properties of IMEX solutions to reaction-diffusion applications.

The next section introduces the prototype two chemical reaction-diffusion problem. Subsequent sections develop theory for computing this problem and demonstrate stability results for a simple application.

5.1 Reaction-Diffusion Systems

We now consider the general two chemical reaction-diffusion system

$$
\begin{align*}
    u_t &= f(u, v) + \nu_1 \Delta u, \quad \nu_1 > 0 \\
    v_t &= g(u, v) + \nu_2 \Delta v, \quad \nu_2 > 0
\end{align*}
$$

(5.41)

where the scalar functions $u$ and $v$ represent chemical concentrations and $f$ and $g$ are nonlinear. Generalization to larger systems is straightforward.

To approximate the system (5.41) using an explicit algorithm frequently necessitates unreasonably small time steps, due to the diffusive terms. An implicit algorithm, however, must contend with the expense and complexity of solving a nonlinear system at each time step. We hope to avoid these problems by treating the nonlinear terms explicitly and the diffusive terms implicitly, using IMEX schemes.
To demonstrate how IMEX solutions to the system (5.41) differ from those of convection-diffusion, linearize (5.41) about the steady state \((u_0, v_0)\) to obtain

\[
\begin{align*}
    u_t &= f_u(u_0, v_0)(\tilde{u}) + f_v(u_0, v_0)(\tilde{v}) + \nu_1 \Delta u + \mathcal{O}(\tilde{u}^2) + \mathcal{O}(\tilde{u}\tilde{v}) + \mathcal{O}(\tilde{v}^2) \\
    v_t &= g_u(u_0, v_0)(\tilde{u}) + g_v(u_0, v_0)(\tilde{v}) + \nu_2 \Delta v + \mathcal{O}(\tilde{u}^2) + \mathcal{O}(\tilde{u}\tilde{v}) + \mathcal{O}(\tilde{v}^2)
\end{align*}
\]

where \(\tilde{u} = u - u_0\) and \(\tilde{v} = v - v_0\). The matrix

\[
\begin{bmatrix}
    f_u(u_0, v_0) & f_v(u_0, v_0) \\
    g_u(u_0, v_0) & g_v(u_0, v_0)
\end{bmatrix}
\]

or simply

\[
\begin{bmatrix}
    f_u & f_v \\
    g_u & g_v
\end{bmatrix}
\]

has eigenvalues

\[
\lambda_{1,2} = \frac{f_u + g_v \pm \sqrt{(f_u + g_v)^2 + 4f_v g_u - 4f_u g_v}}{2}.
\]

Thus an IMEX approximation to (5.41) will most likely require the explicit treatment of eigenvalues with nonzero real parts. For example, in morphogenesis applications,

\[
\text{Re}(\lambda_{1,2}) < 0
\]

for the possibly complex eigenvalues, \(\lambda_{1,2}\), because two of the conditions for generating spatial patterns by a two chemical mechanism (see Murray[16]) are

\[
\begin{align*}
    f_u + g_v &< 0, \\
    f_v g_u - f_u g_v &< 0.
\end{align*}
\]

The spatial patterns which can form in these examples arise from the coupling of diffusion and reaction terms. See Murray[16] or the pioneering work by Turing[21] for detailed derivations of this mechanism.

The next section examines how to integrate equations for which the property (5.43) holds.
5.2 Treatment of Reaction Terms

To determine methods for the efficient integration of reaction-diffusion problems, we consider the explicit case $\nu_1 = \nu_2 = 0$. Stability properties of the explicit extrapolation are examined for first, second and third order SBDF as well as CNLF and CNAB. Methods are sought which possess large stability regions which can accommodate eigenvalues with negative real parts. For this purpose, stability contours for the prototype equation $\dot{x} = (i\beta + \alpha)x$ are derived as in Section 2.10. These are displayed in Figures 5.35 to 5.37.

The contours for leap frog are not displayed because only values on the $\beta$-axis are stable. The corresponding IMEX scheme, CNLF, should not be used for reaction-diffusion because of leap frog's inability to deal with nonzero real eigenvalues.

The contours for second order Adams-Bashforth are displayed in Figure 5.35. The stability region for this scheme includes values which are not purely imaginary. Thus the corresponding second order IMEX schemes (e.g. CNAB and modified CNAB) are better choices for computing reaction-diffusion problems than CNLF.

The contours for the explicit extrapolation used in SBDF are plotted in Figure 5.36. Since this stability region is significantly larger than the region for second order Adams-Bashforth, larger stable time steps should be possible when applying SBDF to reaction-diffusion problems.

The contours for the explicit extrapolation used for third order SBDF are plotted in Figure 5.37. This region is smaller than for the second order case, so we expect third order SBDF to possess a more severe time stepping restriction. This stability region contains the $\beta$-axis, however, so eigenvalues near the $\beta$-axis may be more efficiently handled by this method.

Finally we consider Forward Euler, the extrapolation for all first order methods. Applying this scheme to $\dot{x} = (\alpha + i\beta)x$ yields a stability region consisting of all $\alpha$ and $\beta$
such that

$$|1 + i\beta k + \alpha k| \leq 1$$

which implies that

$$(\alpha + \frac{1}{k})^2 + \beta^2 \leq \frac{1}{k^2}.$$ (5.44)

Thus the stability region is bounded by the circle, centre $(\alpha, \beta) = (-1/k, 0)$, radius $1/k$. Since this region is larger than any of the methods described above, we expect first order SBDF to allow the largest stable time steps for reaction-diffusion problems.

Throughout this section, stability effects from the viscous term are neglected. To verify the usefulness of this simplified stability analysis, numerical experiments for a reaction-diffusion problem are carried out in the next section.
Figure 5.36: Stability Contours for the Explicit Extrapolation of SBDF

Figure 5.37: Contours for the Explicit Extrapolation of 3rd Order SBDF
5.3 Computations

5.3.1 The Schnackenberg System

For our model problem we consider the one-dimensional Schnackenberg system (see Schnackenberg[18]),

\[
\begin{align*}
    u_t &= d(a - u + u^2v) + u_{xx} \\
    v_t &= d(b - u^2v) + \nu v_{xx}
\end{align*}
\]  

(5.45)

having periodic boundary conditions on the interval [0,1].

This model has been used by Murray[16] in the context of morphogenesis. To consider pattern formation consistent with morphogenesis we use the initial conditions

\[
\begin{align*}
    u(x, 0) &= a + b + 0.0004 \sum_{j=1}^{5} \frac{\cos(2\pi j x)}{j} \\
    v(x, 0) &= \frac{b}{(a + b)^2} + 0.0004 \sum_{j=1}^{5} \frac{\cos(2\pi j x)}{j}.
\end{align*}
\]

These initial perturbations from the steady state

\[(\bar{u}, \bar{v}) = (a + b, \frac{b}{(a + b)^2})\]

represent the random modal frequencies that could be present in a biological system.

We select parameters

\[
\begin{align*}
    a &= 0.2 \\
    b &= 2.0
\end{align*}
\]

and

\[
\begin{align*}
    d &= 300.
\end{align*}
\]
Chapter 5. Reaction-Diffusion Experiments

From Murray[15], spatial patterns can be generated using these parameter values. Having selected $a$, $b$ and $d$, an upper bound for the time step size assuming no diffusion can be determined. The Jacobian matrix (5.42) evaluated at $(\bar{u}, \bar{v})$ has approximate eigenvalues $-603 \pm 268i$ for these parameters. Using (5.44), the time step size, $k$, will have to be taken less than about $0.0027$ to ensure that the eigenvalues lie inside the stability region for first order SBDF at $t = 0$.

Computations are carried out for $60 \leq \nu \leq 160$. For $\nu < 60$, spatial error overwhelms time stepping error because patterns form very slowly or not at all. For $\nu > 160$, the qualitative behaviour of the final patterns is similar to that of $\nu = 160$.

There are two qualitatively different solutions. In Figures 5.38 and 5.39, results for $\nu = 60$ are provided for $u$ and $v$. In Figures 5.40 and 5.41, the results for $\nu = 160$ are displayed. These computations are accurate to within $1\%$ of the exact solution and use first order SBDF with fourth order centred differences spatially. The discretization step sizes are $k = 0.0005$ in time and $h = 0.05$ in space.

In the next section, several stability properties for IMEX schemes are demonstrated for the system (5.45).

5.3.2 One-Dimensional Computations

To illustrate stability properties for IMEX schemes, solutions for the model problem (5.45) were computed using discretization step sizes $h = 0.05$ in space and $k = 0.00025$ in time. Using several IMEX schemes, computations are performed to time $t = 0.8$ using fourth order centred (5-point) differences in space.

The max norm relative errors for these schemes are computed by comparing results to those for SBDF using $h = 0.0125$ and $k = 0.00003125$. The resultant errors are plotted against $\nu$ for $100 \leq \nu \leq 160$ in Figure 5.42. For $60 \leq \nu \leq 100$ the errors for all methods except CNLF overlap since spatial error dominates.
Figure 5.38: Concentration, $u$, at $t = 0.8$ for $\nu = 60$

Figure 5.39: Concentration, $v$, at $t = 0.8$ for $\nu = 60$
Figure 5.40: Concentration, $u$, at $t = 0.8$ for $\nu = 160$

Figure 5.41: Concentration, $v$, at $t = 0.8$ for $\nu = 160$
Chapter 5. Reaction-Diffusion Experiments

For $60 \leq \nu \leq 160$, CNLF is unstable as predicted by the theory. This method is unstable even for $k = 2.5 \times 10^{-6}$. CNAB, modified CNAB and third order SBDF produce large errors over much of the interval. First order SBDF and SBDF appear stable over the entire interval. The error for first order SBDF is not plotted because it nearly overlaps that for SBDF.

To determine the nature of the errors, computations for $\nu$ when $\nu = 160$ are plotted in Figure 5.43. From Figure 5.42, the SBDF computation is nearly exact. CNAB, modified CNAB and third order SBDF all have incorrect amplitudes. Furthermore, the dominant modal frequency for third order SBDF and CNAB is not that of the exact solution. Similar effects occur even for initial perturbations 100 times larger.

From Figure 5.44, even for a smaller value of $h$, $h = 1/80$, the results are qualitatively similar. The error for modified CNAB is not plotted because it nearly overlaps that of third order SBDF. In practice, the value of $h$ would not usually so small for these values of $\nu$ because the coarser mesh, $h = 1/20$, yields an error of less than 1% using first order SBDF.

An increase in the time step size to $k = 0.0005$ leaves the error for first order SBDF essentially unchanged, whereas SBDF has an error greater than 35% for $\nu \geq 120$. As predicted by the theory, the method with the largest explicit stability region allows the largest stable time steps.

The results of this section are consistent with the hypothesis that numerical methods possessing large stability regions in the absence of diffusion are preferred for reaction diffusion problems. This is because even for small values of $h$ it is possible for reaction terms to dominate diffusion if parts of the solution are linear in $x$. To illustrate this behaviour, consider the Schnackenberg system (5.45) with $a = b = 0$ and $d = 360$, subject to periodic boundary conditions and initial conditions $u(x,0) = u_0$ and $v(x,0) = 0$. 

Figure 5.42: Relative Errors for Several IMEX Schemes for Various \( \nu \) and \( h = \frac{1}{20} \)

Applying second order centred differences and first order SBDF to this system yields,

\[
\frac{u_j^{n+1} - u_j^n}{k} = -300u_j^n + \frac{u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^{n+1}}{h^2}.
\]

By symmetry, \( u_{j-1}^{n+1} = u_j^{n+1} = u_{j+1}^{n+1} \), thus we obtain

\[
u_j^{n+1} = (1 - 300k)u_j^n,
\]

which implies the stability time step restriction of \( k = \frac{1}{150} \) for any \( h \). This is the same restriction that occurs without diffusion.

The next section considers the two-dimensional case.

5.3.3 Two-Dimensional Computations

For our next problem, we consider the two-dimensional Schnackenberg system

\[
\begin{align*}
    u_t &= 300(0.2 - u + u^2v) + \Delta u \\
    v_t &= 300(2.0 - u^2v) + 120\Delta v.
\end{align*}
\] (5.46)
Figure 5.43: IMEX Computations for $v$, at $t = 0.8$ for $\nu = 160$

Figure 5.44: Relative Errors for Several IMEX Schemes for Various $\nu$ and $h = \frac{1}{80}$
subject to periodic boundary conditions on the interval \( \Omega = [0,1] \times [0,1] \) and initial conditions

\[
\begin{align*}
    u(x,y,0) &= 2.2 + 0.001 \sum_{j=1}^{8} \frac{\cos(2\pi j(x+y))}{j} \\
v(x,y,0) &= 0.41322 + 0.001 \sum_{j=1}^{8} \frac{\cos(2\pi j(x+y))}{j}.
\end{align*}
\]

The problem (5.46) was computed to time \( t = 0.2 \) using discretization step sizes \( h = 1/32 \) in space and \( k = 0.001 \) in time. The standard 5-point Laplacian was used to approximate the diffusion terms. A multigrid solution to the implicit equations was performed using \( V(1,1) \) cycles with one iteration per time step. The components of this iterative algorithm are described in Section 4.3.

Using first order SBDF, this computation has a max norm relative error of less than 0.44\% when compared to a computation with SBDF using \( k = .0001 \) and \( h = \frac{1}{128} \). The plot of \( u \) for this computation is displayed in Figure 5.45. Similar to the one-dimensional case, SBDF, third order SBDF, CNAB and modified CNAB all produce relative max norm errors greater than 1 for this value of \( k \). Refining the time step to \( k = 0.0005 \) produces errors of less than 0.44\% for SBDF and first order SBDF. Modified CNAB, CNAB and CNLF still produce relative errors greater than 1. All the methods except CNAB and CNLF have errors of less than .44\% when the time step \( k = 0.00025 \) is used. The results for the refined mesh, \( h = 1/64 \), are qualitatively similar.

Using the results from this and previous sections, a description of how to choose IMEX schemes for reaction-diffusion problems is presented next.

5.4 Choice of IMEX Scheme

Based on the observations in this and previous chapters we provide a few guidelines for selecting IMEX schemes for reaction-diffusion problems. These ideas can also be applied
Figure 5.45: Concentration, $u$, at $t = 0.2$ for $\nu = 120$
to problems where explicitly treated terms have eigenvalues with negative real parts whose size is not small compared to the implicitly treated terms.

The primary observation is that CNLF should not be used in reaction-diffusion problems. This scheme cannot accommodate the real eigenvalues of the reaction term, and will likely become unstable.

SBDF methods are excellent choices for reaction-diffusion problems. These methods allow large time steps in comparison to other methods of the same order because their explicit extrapolations include more of the negative $\alpha$-axis than other schemes of the same order.

Finally, application of an IMEX scheme of lower order than the spatial discretization should be considered. Lower order methods allow larger time steps because their explicit extrapolations tend to possess larger stability regions.
Chapter 6

Conclusions

From the analysis and experiments of the previous four chapters, several conclusions and recommendations for future work are made. These are given in the next two sections.

6.1 Results

The analysis of the general, linear multistep IMEX scheme demonstrates that $s$-step IMEX schemes can have at most order $s$ accuracy, and that such schemes form an $s$-parameter family of methods. This fact leads us to consider only $s$-step, order $s$ schemes throughout this thesis.

A parameterization for first order, one-step schemes was given. Of these methods, first order SBDF (2.15) was recommended because it allows large stable time steps for $\nu \gg 1/k$ and produces a strong asymptotic decay of high frequency spatial modes.

A parameterization for second order, two-step schemes was given. Included in this two-parameter family of schemes are CNLF (2.19), CNAB (2.17), SBDF (2.20) and our newly proposed scheme, modified CNAB (2.18). An analysis for the linear advection-diffusion equation showed that for small mesh Reynolds numbers (2.24), $R < 2$, SBDF produces the strongest asymptotic decay of high frequency spatial modes and allows the largest stable time steps. CNLF was shown to allow the largest stable time steps for large mesh Reynolds numbers, $R > 2$. The modified CNAB scheme is recommended for the small mesh Reynolds number case when a small truncation error along with a strong decay of high frequency error modes is desired.
For the third order case, a three-parameter family of three-step schemes was given. It was shown that third order SBDF (3.26) produces the strongest asymptotic decay of these schemes and that it is stable for all $\nu \geq 0$. For any $\nu \geq 0$, however, one of CNLF or SBDF allows larger stable time steps. A fourth order scheme, fourth order SBDF (3.36) was also given. This scheme was shown to be stable for all $\nu \geq 0$. It possesses an even more severe time-stepping restriction than third order SBDF.

Computations for solutions to a variable coefficient problem were carried out using second order, centred differences spatially. Several of the previously identified theoretical results were demonstrated. In particular, SBDF allowed the largest stable time steps for small mesh Reynolds numbers and CNLF allowed the largest stable steps for large mesh Reynolds numbers. The errors for CNAB and modified CNAB were very similar, supporting the claim that these methods have similar truncation errors. Stability for modified CNAB was also similar to CNAB. Third order SBDF was shown to possess a more severe time-stepping restriction than many second order methods. Nonetheless, this method is recommended when high accuracy is needed because it produces a much smaller error than second order schemes when stable.

Based on solutions for a nonlinear problem we conclude that CNLF, third and fourth order SBDF perform well for the zero viscosity case. Of these schemes, CNLF was non-dissipative while third order SBDF was the most strongly dissipative. Other second order schemes should be avoided in this case.

Using Chebyshev and Fourier spectral collocation, solutions to the Burgers equation for small to moderate mesh Reynolds numbers were computed using various IMEX schemes. For these problems, CNLF had a very severe time step restriction. These computations also suggest that SBDF had the mildest time step restriction of the methods considered. Although it had a more severe time-stepping restriction than many second order schemes, third order SBDF appeared to be useful when high accuracy was required.
Chapter 6. Conclusions

Further pseudospectral computations for the Burgers equation demonstrated that a strongly damping time-stepping scheme such as SBDF, modified CNAB or third order SBDF can be used to inexpensively reduce aliasing. Application of a weakly damping scheme such as CNLF or CNAB in poorly spatially resolved, aliased computations is discouraged.

Using a multigrid method to solve the implicit equations, solutions to the 2D convection-diffusion equation for small mesh Reynolds numbers were computed using various IMEX schemes. These results clearly demonstrate that use of a strongly damping time-stepping scheme may lead to fewer fine grid iterations in multigrid than use of a weakly damping scheme. In particular, use of SBDF or modified CNAB produced a more efficient multigrid method than did use of CNLF or CNAB. The idea of using a strongly damping time-stepping scheme to reduce the number of iterations in multigrid should also extend to fully implicit schemes.

The reaction-diffusion problem was considered. For this problem, it is demonstrated that schemes which possess large stability regions in the absence of diffusion are preferred. Such schemes are best able to cope with the growth associated with the reaction terms. Of the IMEX schemes considered, first order SBDF allowed the largest time steps and second order SBDF allowed the largest stable time steps of second order schemes. Use of CNLF is strongly discouraged in reaction-diffusion problems.

Perhaps the most surprising conclusion of this study is the poor showing of the most popular scheme currently in practice, namely CNAB. In particular, our newly proposed modified CNAB scheme (2.18) appears to supersede CNAB because it almost always performed as well as, or much better than, CNAB.
6.2 Future Work

There are many opportunities for future work in IMEX schemes.

An investigation to determine when IMEX schemes are more efficient than fully explicit or fully implicit schemes would be of interest. For the convection-diffusion case an analysis to determine when a fully explicit treatment is competitive is especially needed. For this case, we expect fully explicit schemes to be more efficient for very large mesh Reynolds numbers because the time-stepping restriction arises primarily from the convection term.

A study of the constant of the truncation error for IMEX schemes would be very interesting, especially for the second order case. Such an analysis would help determine which second order scheme to apply to a particular problem. However, this is far less simple than for usual ODE multistep schemes.

It is clear that algorithms using IMEX schemes are easier to implement than those using fully implicit schemes in reaction-diffusion problems. We have not considered how efficient IMEX schemes are in comparison to fully implicit schemes for these systems. A study making this comparison would be of interest.

The analysis of this thesis has focussed on the finite difference case. Because the eigenvalues for spectral methods are different than for finite differences as is their meaning, we suspect that parts of the theory will not apply to spectral methods. For this reason, an analysis of the linear advection-diffusion equation for Chebyshev and Fourier spectral methods would be useful.

Future work in time-dependent multigrid is also needed. This thesis has only examined the small mesh Reynolds number case. The large mesh Reynolds number case should be examined because it may also yield interesting behaviour.

Throughout this work, periodic boundary conditions were assumed. In practice, we
usually have to impose non-periodic boundary conditions. An analysis to determine stable methods of imposing Dirichlet and Neumann boundary conditions for IMEX schemes would be very useful.

This thesis has applied a one-step scheme, first order SBDF, with a very small time step to obtain the starting values in multistep IMEX schemes. A study to determine simple, efficient methods for obtaining these initial values would be of interest.

Further analysis of third and fourth order schemes is also possible. For example, it would be desirable to determine if schemes exist which allow significantly larger stable time steps than third or fourth order SBDF schemes.

For systems which are strongly convective, the phase lag can dominate the error. An analysis of this source of error for IMEX schemes should also be carried out.

Finally, we have only considered the constant time step size case. In practice, variable time-stepping algorithms are often preferred. A study to examine how to implement variable time-stepping for various IMEX schemes would be interesting.
Bibliography


