Final Year Project Final Report

William Bolton - 1300316

Department of Mathematics, University of Warwick, Coventry CV4 7AL, United Kingdom

We describe and analyse the theory behind two kinds of finite difference scheme, Dispersion Relation Preserving (DRP) schemes and Summation By Parts (SBP) schemes, paying particular attention to the benefits of each in the context of acoustical problems. We then look to construct a sixth order approximation scheme for the first derivative, which combines all of the beneficial properties found and outline the systematic method taken. The procedure leads us to a set of non-linear equations which remain to be solved but implicitly define the structure the scheme would need to take in order to meet the SBP criteria. The scheme could then be optimized in a DRP like fashion.

I. Introduction

Computational aeroacoustics (CAA) is an area of particular industrial interest as developments can lead to better simulation of sound propagation. Modern computers have facilitated the direct computational simulation of acoustical problems; this is a powerful tool with many potential applications including engineering quieter vehicles, simulating sound propagation into the atmosphere and designing musical instruments. The volume of noise produced by vehicles, particularly aircraft, is heavily regulated [1, 2] and new standards governing the legal threshold for noise produced continue to be introduced [3] which further necessitate the study.

To computationally model the equations which govern aeroacoustics, approximations to the first derivative are frequently required. The formal definition of the first derivative is given by:

$$u'(x) = \lim_{\Delta x \to 0} \frac{u(x+\Delta x) - u(x)}{\Delta x} \tag{1}$$

Since computers are unable to exactly compute limits to zero, many discrete, finite difference approximation schemes exist to approximate derivatives computationally. Additional difficulty arises from the fact that in the realm of aeroacoustics singularities and discontinuities are common due to the frequency of phenomena such as shocks and blow ups.

Currently a lot of effort is being put into developing finite difference schemes for derivatives in ways which ensure the physics of the wave propagation are preserved [4]. Many such physical properties depend on the dispersion relation of the wave, that i0,s the relationship between the wave number and frequency. However, conventional finite difference schemes are often poor at preserving these properties.

Dispersion Relation Preserving (DRP) schemes have been developed to deal with exactly this problem. Unfortunately, although many of these schemes have been shown to perform well for waves of constant amplitude, they under-perform when applied to waves with varying amplitudes. Furthermore, the methods these schemes use break down at the domain boundaries where the schemes are often unstable [5, 6].

Another class of schemes known as Summation by Parts (SBP) schemes have been show to be both well-posed and provably stable [4] as they exhibit a property similar to integration by parts which allows stability to be proven via an energy method. This property then allow us to weakly impose boundary conditions by using the method of Simultaneous Approximation Terms (SATs) [7].

The aim of this project is to understand the theory behind, and then investigate the strengths and weaknesses of the both kinds of finite difference scheme and then develop and combine the techniques to make new schemes which improve on existing schemes. We then determine that it is not possible to construct a pentadiagonal, sixth order accurate, 7 point, implicit scheme with the SBP property, but that it is possible to create a new tridiagonal scheme with those properties. Furthermore, we show that such a scheme could be developed into a DRP scheme.

II. Theory

A. Preliminaries and Notation

We let our domain be split into a grid with $N+1$ equally spaced grid points indexed from 0 to N. Our focus is on centred schemes for the first derivative which are symmetric about the point which the derivative is to be found at. We define Δx as the grid spacing such that: $x_i = i\Delta x$, $u_{i+1} = u(x_i + \Delta x)$, with $u_i = u(x_i)$. By manipulating various Taylor series we derive approximations to the first derivative using linear combinations of the function values at various local grid point. In general for a central scheme defined on the interior of the domain, with a n point stencil which is $2M+1$ diagonal we set:

$$u_i' + \sum_{j=1}^{M} \beta_j (u_{i+j}' + u_{i-j}') \approx \frac{1}{\Delta x} \sum_{j=1}^{\frac{n-1}{2}} a_j \left(\frac{u_{i+j} - u_{i-j}}{2j} \right). \tag{2}$$

By considering this as one equation per each grid point we can also write (2) as a matrix equation:

$$P\mathbf{u}' = \frac{1}{\Delta x} Q\mathbf{u} \tag{3}$$

Where P and Q are $n \times n$ matrices and $\mathbf{u}$ and $\mathbf{u}'$ are n dimensional vectors representing the function and its derivative at each grid point. We note here that P will have $1s$ on the diagonal and be symmetric, and Q will be asymmetric.

The relations between the coefficients β_j and a_j are found by matching terms with the coefficients of Taylor series of various orders and will be referred to as accuracy conditions. The first unmatched coefficient of the Taylor expansion determines the formal truncation error. To achieve higher orders of approximation (lower truncation error) more linear relations, found by including higher order Taylor terms, are required to be satisfied. Schemes that match $\gamma = n + 2M - 1$ terms in the Taylor expansion, which is the highest possible [5], are known as Maximal Order (MO) schemes. The relations for pentadiagonal, 7-point schemes, up to 10th order are detailed By Lele in (2.1.1)-(2.1.5) [8]. In periodic cases, the system of equations can be written together as a linear system for unknown derivative values. Lower order approximations where fewer equations must be satisfied leave more degrees of freedom in the solution so that there are many possible choices of coefficients.

We are able to choose values for some of the (a_j) terms to simplify the computation, for example, in a 7-point, pentadiagonal, 4th order family of schemes, we have:

$$\beta_2(u_{i-2}' + u_{i+2}') + \beta_1(u_{i-1}' + u_{i+1}') + u_i' = a_3 \frac{u_{i+3} - u_{i-3}}{6\Delta x} + a_2 \frac{u_{i+2} - u_{i-2}}{4\Delta x} + a_1 \frac{u_{i+1} - u_{i-1}}{2\Delta x}$$

and using our 5 parameters we must satisfy two relations between the coefficients to achieve 4th order accuracy [8] so we have 3 degrees of freedom. If we were to require 6th order accuracy, we would have three relations to satisfy, leaving us with only two degrees of freedom. There are many ways we can benefit from these degrees of freedom; one choice we could make would be to set $\beta_2 = 0$ (or equivalently, $M = 1$) to generate 3-point diagonal schemes which will be simpler to compute, if we set $\beta_1 = \beta_2 = 0$ (or $M = 0$), we would have an explicit scheme. We could also choose to set $a_3 = 0$ which would mean we would only need a 5 point stencil.

Near the boundaries (for a non-periodic case), conventional symmetric schemes break down as we run out of grid points and need additional relations to impose the problem's boundary conditions. Here it is common to use asymmetric finite difference schemes with forward or backwards projection. This means we get boundary blocks at the edges of our scheme which are not $2M + 1$ point diagonal and are often unstable. The coefficients at these boundary blocks are determined by the boundary conditions of the problem. The instability of boundary schemes poses problems for real life modelling as it leads to inaccuracies.

Schemes can be implicit or explicit. An explicit scheme is when $\beta_j = 0$ for all j, the major advantage of this are that the solution algorithm is very simple to set up and the computational time to solve is usually less as it's not necessary to complete large matrix manipulations at every step. However, for a given Δx, explicit schemes require a large number of points per wavelength in order to be accurate. Implicit schemes, though more computationally demanding require fewer points per wavelength so a larger value of Δt may be used. The stability of explicit and implicit methods and the constraints on Δx and Δt are analysed in [9].

B. Dispersion Relation Preserving Schemes

Instead of only using the formal truncation error to quantify the error in an approximation scheme, it is desirable to quantify the approximation error by comparing the Fourier transform of the approximate derivative to that of the original derivative, this equates to comparing their dispersion relations. We can do this comparison by utilizing the property that the wave number of a derivative is proportional to the wave number of the original function [8, 10]. If the Fourier transforms are similar we ensure that the dispersiveness, damping rate, isotropy, anisotropy, group velocity and phase velocity (which are all determined by the dispersion relation) are preserved. If we assume our function is a constant amplitude wave of the form $u(x) = \Re(Ae^{i\theta x}) = Acos(\theta x)$ with derivative

$u'(x) = \Re(i\theta A e^{i\theta x})$. Starting from (2) and taking real parts we have

$$\theta A e^{i\theta x} + \sum_{j=1}^{M} \beta_j \theta A \left(e^{i\theta(x+j\Delta x)} + e^{i\theta(x-j\Delta x)}\right) \approx \frac{1}{\Delta x} \sum_{j=1}^{\frac{n-1}{2}} a_j A \left(\frac{e^{i\theta(x+j\Delta x)} - e^{i\theta(x-j\Delta x)}}{2j}\right)$$

$$\theta A e^{i\theta x} + \theta A e^{i\theta x} \sum_{j=1}^{M} \beta_j \left(e^{i\theta j\Delta x} + e^{-i\theta j\Delta x}\right) \approx \frac{A e^{i\theta x}}{\Delta x} \sum_{j=1}^{\frac{n-1}{2}} a_j \left(\frac{e^{i\theta j\Delta x} - e^{-i\theta j\Delta x}}{2j}\right)$$

$$\theta + \theta \sum_{j=1}^{M} 2\beta_j cos(\theta j\Delta x) \approx \frac{1}{\Delta x} \sum_{j=1}^{\frac{n-1}{2}} a_j \left(\frac{isin(\theta j\Delta x)}{j}\right).$$

Rearranging and absorbing the $\frac{i}{j}$ into a_j, we reach

$$\theta\Delta x = \frac{\sum_{j=1}^{\frac{n-1}{2}} a_j sin(\theta j\Delta x)}{1 + 2\sum_{j=1}^{M} \beta_j cos(\theta j\Delta x)}. \tag{4}$$

We use this to make the comparison and then choose our coefficients to ensure that these two values are similar. For example, Tam and Webb [10] chose to minimise this error quantity:

$$E = \int_{\frac{-\pi}{2}}^{\frac{\pi}{2}} |i\kappa - \sum_{j=1}^{\frac{n-1}{2}} \beta_j e^{ij\kappa}|^2 dk$$
$$\text{with } \kappa = \theta\Delta x.$$

The exact choice of error quantity used will depend on the specific problem being solved, and the geometry involved.

While Maximal Order schemes have low truncation errors, they often perform poorly at minimising the dispersion error. Dispersion Relation Preserving (DRP) schemes, initially proposed by Tam and Webb in [10], aim to deal with this by sacrificing the truncation error and choosing coefficients which minimise the dispersion error. In constructing DRP schemes we elect to match a lower number, L, of Taylor coefficients. This leaves $\gamma - L$ degrees of freedom which we can use to optimize the wave number by minimising our chosen error quantity with respect to the spare coefficients. Such schemes require fewer points per wavelength to accurately resolve constant amplitude waves [6]. However, we still have the same problems at the boundaries as before however so still need to use a different approach at the exterior of the scheme.

It is worth noting that when θ is complex (equating to an exponentially growing or decaying wave), it has been shown that Maximal Order schemes do better than DRP schemes at optimizing $\bar{\theta}$ despite the fact that DRP schemes have been designed for this purpose [6]. This is because DRP schemes are sensitive to the value of $arg(\theta\Delta x)$ whereas Maximal Order schemes are not. This means for Maximal Order schemes the number of points per (complex) wavelength can just depend on the magnitude $|\theta\Delta x|$ but for DRP schemes this doesn't work as it is necessary to know exact complex wavenumbers in all directions. Unfortunately the 1D advection equation, which has frequently been used to test the performance of DRP schemes, has constant wave amplitude which means the flaws noted in [6] were not demonstrated until more recently. This means the study of schemes outlined here is only applicable for problems with real wave numbers.

C. Summation By Parts Schemes

While it is easy to derive higher order finite difference schemes on the interior of the domain, and relatively simple to introduce an extra degree of freedom in order to make the interior into a DRP scheme, it is non-trivial to find stable high order finite difference schemes close to the boundaries. If we can establish the existence of an upper bound for our approximate solution, then we can establish the uniqueness of our solution proving that our problem is well posed (providing we have some initial condition) [11]. Our proof of the necessary properties for this upper bound to exist is based on an energy method by which we bound our solution [7]. In general a homogeneous initial value problem with $g_0(t) = g_1(t) = 0$ is written as:

$$u_t = R(x, t, \partial_x)u + F, \qquad 0 \leq x \leq 1, \qquad t \geq 0 \tag{5}$$

$$u(x, 0) = f(x), \tag{6}$$

$$L(t, \partial_x)u(0, t) = g_0(t), \tag{7}$$

$$L(t, \partial_x)u(1, t) = g_1(t), \tag{8}$$

where R and L are differential operators defining the problem and boundary conditions, and $F = F(x, t)$ is a forcing term, can be shown to be well posed if it satisfies an estimate similar to this [12]:

$$||u||^2 \leq Ke^{kt}||f|| \qquad \forall f \in C_c^{\infty} \tag{9}$$

Where K and k are constants independent of f. This requires appropriate boundary conditions to be chosen to guarantee a unique smooth solution exists.

We now consider the homogeneous 1D advection equation, with some scalar field

$u(x,t)$ with positive unit wave speed, as an example:

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0, \qquad 0 \le x \le l, \qquad u(0,t) = 0, \qquad u(l,0) = u_L, \qquad t \ge 0 \tag{10}$$

The rate of change of energy E with respect to time is:

$$\frac{dE}{dt} = -2\int_0^l u\frac{\partial u}{\partial x}dx$$

Applying integration by parts yields:

$$\frac{d}{dt}\int_0^l u^2 dx = -u_L^2 \le 0 \tag{11}$$

Therefore the problem is bounded and so with initial conditions is well posed [13] and has a unique, smooth solution.

We now write an arbitrary finite difference scheme in matrix notation and consider a discretization of the homogeneous advection equation (10). Let:

$$PD\boldsymbol{u} = Q\boldsymbol{u} \tag{12}$$

Where D is an operator representing the first derivative. We want to find P and Q (if they exist) such that:

$$\frac{\partial \boldsymbol{u}}{\partial x} \approx P^{-1}Q\boldsymbol{u}$$

Then (10) becomes:

$$\boldsymbol{u}_t + D\boldsymbol{u} = 0, \qquad x_0 = 0 \qquad x_n = l, \qquad u_0(t) = 0, \qquad u_n(0) = u_L, \qquad t \ge 0 \tag{13}$$

We pick P to be positive definite so that it defines an inner product with:

$$\langle \boldsymbol{u}, \boldsymbol{v} \rangle_P = \boldsymbol{u}^T P \boldsymbol{v} \tag{14}$$

$$||\boldsymbol{u}||^2 = \boldsymbol{u}^T P \boldsymbol{u} \tag{15}$$

$$\int_{x_L}^{x_R} uv dx \approx \boldsymbol{u}^T P \boldsymbol{v} = \langle \boldsymbol{u}, \boldsymbol{v} \rangle_P \tag{16}$$

and Q such that:

$$Q + Q^T = E_n - E_0 = diag[0, ..., 0, 1] - diag[1, 0, ..., 0] \tag{17}$$

Where E_i are matrices who have 1 as the ith value of their diagonal and are zero elsewhere. We see that when (14)-(17) hold, a property similar to integration by parts - known as summation by parts (SBP) - also holds. The integration by parts formula for is:

$$\int_\Omega uv dx = uv|_\Omega - \int_\Omega v\frac{\partial u}{\partial x}dx \tag{18}$$

The discrete analog of this which (14)-(17) are necessary and sufficient for [8] is:

$$\langle \boldsymbol{u}, \boldsymbol{Dv} \rangle_P = \boldsymbol{u}^T (E_n - E_0)\boldsymbol{v} - \langle P^{-1}Q\boldsymbol{u}, \boldsymbol{v} \rangle_P \tag{19}$$

This implies that an approximation scheme with conditions (14)-(17) will yield the same energy estimate for the 1D, homogeneous advection equation as the analytical approach, proving the approximation is time stable [7]:

$$\begin{aligned} \frac{d\boldsymbol{u}^T P \boldsymbol{u}}{dt} &= \boldsymbol{u}^T P \frac{d\boldsymbol{u}}{dt} + \frac{d\boldsymbol{u}^T}{dt} P \boldsymbol{u} & &= -\boldsymbol{u}^T (Q + Q^T)\boldsymbol{u} \\ &= -\boldsymbol{u}^T (E_n - E_0)\boldsymbol{u} & &= -(u_n^2 - u_0^2) \\ &= -u_L^2 & &\leq 0 \end{aligned}$$

The general method for constructing specific SBP schemes is to begin with a stencil and then make modifications at the grid points and boundaries to ensure (14)-(17) are satisfied along with the accuracy conditions. This process is well documented in [8] and beyond a certain order will leave degrees of freedom which can then be used for optimization but the optimization must be done in a way that ensures H remains positive definite. Some investigations have been made in using these degrees of freedom to develop joint DRP-SBP schemes. In particular construction of some low order joint SBP-DRP [4, 5] schemes has been achieved. However this area of study remains fairly limited.

We can construct implicit schemes satisfiying a generalisation of the SBP property by multiplying by a matrix H on each side giving:

$$HPD\boldsymbol{u} = HQ\boldsymbol{u}. \tag{20}$$

Then we set $W = HP$ and $V = HQ$ and find H such that W is symmetric and V satisfies (17). The matrices W and V will then contain a generalisation of the interior scheme which can be recovered by multiplication with H^{-1} [14].

D. Simultaneous Approximation Terms

Simultaneous Approximation Terms (SATs) deal with the issues that arise at the boundaries of the scheme and between blocks, however they rely on problem being well posed and stable [7] so are only applicable with stable schemes such as SBP schemes. Solutions in different blocks must be glued together in a way that preserves stability and accuracy. SATs are a method by which we can weakly impose the boundary or block interface conditions whilst preserving stability by introducing additional penalty terms which we add to our problem, they are derived by considering the characteristics at the edges of the domain. This permits us to prove stability for more complicated problems than with SBP schemes alone.

The condition for well posedness established in (9) can be extended to inhomogeneous boundary problems using the transformation:

$$\tilde{u}(x,t) = \begin{cases} u(0,t) - g_0(t) & \text{if } x = 0, \\ u(1,t) - g_1(t) & \text{if } x = 1, \\ u(x,0) - f(x) & \text{if } t = 0. \end{cases} \tag{21}$$

However in order for $\tilde{u}$ to satisfy the initial value problem (5) - (8), we require g_0 and g_1 to be time differentiable. If we replace (9) with:

$$||u||^2 \leq K(t) \left(||f||^2 + \int_0^t (||F(\tau)||^2 + |g_0(\tau)|^2 + |g_1(\tau)|^2 d\tau) \right) \tag{22}$$

with $K(t)$ bounded and independent of F, g_0, g_1 and f. Then the initial value problem is strongly well posed even if g_0 and g_1 are not time differentiable [12]. We recognise (22) as an integration by parts formula. Considering a discretisation in space such that $\boldsymbol{u} = [u_0, u_1, ...u_n]^T$, if we now let D be an operator representing the first derivative. We discretise (5) - (8) as:

$$(u_j)_t = \tilde{R}_j(x_j,t)u_j + F_j + \mathcal{S}_j, \qquad j = 0, ..., n, \qquad t \geq 0, \tag{23}$$

$$u_j(0) = f_j, \tag{24}$$

$$Lu_0(t) = g_0(t), \tag{25}$$

$$Lu_n(t) = g_1(t) \tag{26}$$

Where $\tilde{R}_j$ is the approximation to R_j at x and $\mathcal{S}_j$ is a term added to help impose boundary conditions and will be explained in the next section. Then the discrete analog of (22) is given by:

$$||\boldsymbol{u}(t)||^2 \leq K(t) \left(||f||^2 + \max\, ||F(\tau)||^2 + \max\, ||g_0(\tau)||^2 + \max\, ||g_1(\tau)||^2 d\tau \right) \tag{27}$$

for $\tau \in [0,t]$ [12]. As an example, we consider the 1D advection equation with inhomogeneous boundary conditions:

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0, \qquad 0 \le x \le l, \qquad t \ge 0 \tag{28}$$

$$u(x,0) = f(x) \tag{29}$$

$$u(0,t) = g_0(t) \tag{30}$$

The spatial discretisation of this is given by:

$$\frac{d\boldsymbol{u}}{dt} + D\boldsymbol{u} = P^{-1}\mathcal{S}, \qquad x_0 = 0, \qquad x_n = l, \qquad t \ge 0 \tag{31}$$

$$\boldsymbol{u}(0) = \boldsymbol{f} \tag{32}$$

$$u_n(t) = u(l,t) = u_L(t) \tag{33}$$

Where $\boldsymbol{u} = (u_0(t), u_1(t), ..., u_n(t))^T$ and $\boldsymbol{f} = (f(x_0), ..., f(x_n))^T$ and $\mathcal{S} = (\mathcal{S}_0, 0, ..., 0)^T$ is a vector to enforce the boundary condition $u_0(t) = g_0(t)$ which shall be constructed later. We let $D = P^{-1}Q$ as before and $\mathcal{S}_0 = (\sigma u_0 - g_0)$ where σ is a parameter. Recalling that $\frac{d||\boldsymbol{u}||^2}{dt} = \frac{d\boldsymbol{u}^T P\boldsymbol{u}}{dt}$ We then calculate the same energy estimate as before and find:

$$\begin{aligned}
\frac{d\boldsymbol{u}^T P\boldsymbol{u}}{dt} &= \boldsymbol{u}^T P\frac{d\boldsymbol{u}}{dt} + \frac{d\boldsymbol{u}^T}{dt}P\boldsymbol{u} && = -\boldsymbol{u}^T(Q+Q^T)\boldsymbol{u} + 2\boldsymbol{u}\mathcal{S} \\
&= -\boldsymbol{u}^T(E_n - E_0)\boldsymbol{u} + 2\boldsymbol{u}\mathcal{S} && = -(u_n^2 - u_0^2) + 2u_0\mathcal{S}_0 \\
&= -u_L^2 + u_0^2 + 2\sigma u_0^2 - 2u_0 g_0 && \le u_0^2(1+2\sigma) - 2u_0 g_0
\end{aligned}$$

If $\sigma \le -1/2$ we have [13]:

$$\frac{d||\boldsymbol{u}||^2}{dt} \le -2u_0 g_0 \le 0$$

We must also choose σ such that Gauss' Theorem holds for our discrete operators i.e.

$$\begin{aligned}
(u_L - g_0) &= \int_0^l \frac{\partial u}{\partial x}dx && \approx \langle \mathbf{1}, D\boldsymbol{u}\rangle_P \\
&= \mathbf{1}^T PD\boldsymbol{u} && = \mathbf{1}^T\mathcal{S} - \mathbf{1}^T Q\boldsymbol{u} \\
&= \sigma u_0 - g_0 + u_0 - u_L && \implies \sigma = -1
\end{aligned}$$

so we see that choosing $\sigma = -1$ choice ensures both conservation and stability [7, 13] even with our inhomogeneous boundary conditions.

III. Results

A. Constructing 6th Order, 7 Point implicit SBP Schemes

Whilst a variety of examples of explicit SBP schemes have been found, notably in [13], very few implicit schemes have been found due to the difficulty in solution. The advantage of implicit schemes is that they allow us to use a greater time step than explicit schemes as we need fewer points per wavelength to accurate compute the derivative. Finding a higher order, implicit SBP scheme would also guarantee stability and allow us to impose any boundary conditions using SATs.

Carpenter, Gottlieb and Abarbanel [14], constructed an implicit fourth order scheme with third order accuracy at the boundaries in 1994 but since then there appears to be little further development. Motivated by their approach we now present our steps towards solving the conditions necessary for the construction of a sixth order, implicit, SBP scheme which has fifth order accuracy at the boundaries. Note that we only consider the upper boundary block as we can just take the transpose of this to use for the lower boundary. We wish to construct a scheme of the form:

$$HP\boldsymbol{u}' = HQ\boldsymbol{u}. \tag{34}$$

On the interior of our problem, we use a central difference sixth order scheme with coefficients α, β, a, b, we begin with a pentadiagonal, seven point scheme.

$$\beta(u'_{i-2} + u'_{i+2}) + \alpha(u'_{i-1} + u'_{i+1}) + u'_i = c\frac{u_{i+3} - u_{i-3}}{6\Delta x} + b\frac{u_{i+2} - u_{i-2}}{4\Delta x} + a\frac{u_{i+1} - u_{i-1}}{2\Delta x} \tag{35}$$

The accuracy relations required for sixth order are [8]:

$$a + b + c = 1 + 2(\alpha + \beta) \tag{36}$$

$$a + 2^2 b + 3^2 c = 2 \times 3(\alpha + 2^2\beta) \tag{37}$$

$$a + 2^4 b + 3^4 c = 2 \times 4(\alpha + 2^4\beta) \tag{38}$$

From (34) and (35) we write:

$$P = \begin{bmatrix} p_{0,0} & \cdots & \cdots & p_{0,n} & \cdots & \cdots & \cdots & \cdots & 0 \\ \vdots & \ddots & & \vdots & & & & & \\ \vdots & & \ddots & \vdots & \beta & & & & \\ p_{n,0} & \cdots & \cdots & p_{n,n} & \alpha & \beta & & & \\ \vdots & & \beta & \alpha & 1 & \alpha & \beta & & \\ \vdots & & & \ddots & \ddots & \ddots & \ddots & \ddots & \\ 0 & & & & & & & & \end{bmatrix} \tag{39}$$

$$Q = \begin{bmatrix} q_{0,0} & \cdots & \cdots & \cdots & q_{0,n} & \cdots & \cdots & \cdots & \cdots & 0 \\ \vdots & \ddots & & & \vdots & & & & & \\ \vdots & & \ddots & & \vdots & \frac{c}{6} & & & & \\ \vdots & & & \ddots & \vdots & \frac{b}{4} & \frac{c}{6} & & & \\ q_{n,0} & \cdots & \cdots & \cdots & q_{n,n} & \frac{a}{2} & \frac{b}{4} & \frac{c}{6} & & \\ \vdots & & -\frac{c}{6} & -\frac{b}{4} & -\frac{a}{2} & 0 & \frac{a}{2} & \frac{b}{4} & \frac{c}{6} & \\ \vdots & & & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & & & & & & & & & \end{bmatrix}. \tag{40}$$

And as we are looking for an implicitly defined scheme we look to solve, subject to the SBP conditions, for H which we write as:

$$H = \begin{bmatrix} h_{0,0} & \cdots & \cdots & h_{0,n} & \cdots & \cdots & \cdots & \cdots & 0 \\ \vdots & \ddots & & \vdots & & & & & \\ \vdots & & \ddots & \vdots & x & & & & \\ h_{n,0} & \cdots & \cdots & h_{n,n} & y & x & & & \\ \vdots & & x & y & z & y & x & & \\ \vdots & & & \ddots & \ddots & \ddots & \ddots & \ddots & \\ 0 & & & & & & & & \end{bmatrix} \tag{41}$$

We now introduce some more matrices to simplify the algebra, first arbitrary matrices which we are trying to solve for:

$$\hat{P} = \begin{bmatrix} p_{0,0} & \cdots & p_{0,n} \\ \vdots & \ddots & \vdots \\ p_{n,0} & \cdots & p_{n,n} \end{bmatrix} \qquad \hat{Q} = \begin{bmatrix} q_{0,0} & \cdots & q_{0,n} \\ \vdots & \ddots & \vdots \\ q_{n,0} & \cdots & q_{n,n} \end{bmatrix} \qquad \hat{H} = \begin{bmatrix} h_{0,0} & \cdots & h_{0,n} \\ \vdots & \ddots & \vdots \\ h_{n,0} & \cdots & h_{n,n} \end{bmatrix}.$$

Some simple matrices to facilitate the matrix algebra necessary:

$$A_1 = \begin{bmatrix} 0 & \cdots & \cdots & 0 \\ \vdots & \ddots & & \vdots \\ 0 & & \ddots & \vdots \\ 1 & 0 & \cdots & 0 \end{bmatrix}, \quad A_2 = \begin{bmatrix} 0 & \cdots & \cdots & 0 \\ \vdots & \ddots & & \vdots \\ 1 & & \ddots & \vdots \\ 0 & 1 & \cdots & 0 \end{bmatrix}, \qquad A_3 = \begin{bmatrix} 0 & \cdots & \cdots & \cdots & 0 \\ \vdots & \ddots & & & \vdots \\ 1 & & \ddots & & \vdots \\ 0 & 1 & & \ddots & \vdots \\ 0 & 0 & 1 & \cdots & 0 \end{bmatrix}.$$

And the following matrices which come from the form of (35):

$$C = \begin{bmatrix} 1 & \alpha & \beta & 0 & \cdots \\ \alpha & 1 & \alpha & \beta & \ddots \\ \beta & \alpha & 1 & \alpha & \ddots \\ 0 & \beta & \alpha & 1 & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{bmatrix} \quad D = \begin{bmatrix} z & y & x & 0 & \cdots \\ y & z & y & x & \ddots \\ x & y & z & y & \ddots \\ 0 & x & y & z & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{bmatrix} \quad S = \begin{bmatrix} 0 & \frac{a}{2} & \frac{b}{4} & \frac{c}{6} & 0 & \cdots \\ -\frac{a}{2} & 0 & \frac{a}{2} & \frac{b}{4} & \frac{c}{6} & \ddots \\ -\frac{b}{4} & -\frac{a}{2} & 0 & \frac{a}{2} & \frac{b}{4} & \ddots \\ -\frac{c}{6} & -\frac{b}{4} & -\frac{a}{2} & 0 & -\frac{a}{2} & \ddots \\ 0 & -\frac{c}{6} & -\frac{b}{4} & -\frac{a}{2} & 0 & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}.$$

Now we can write P and Q in blocks in terms of these matrices:

$$P = \left[\begin{array}{c|c} \hat{P} & \alpha A_1 + \beta A_2 \\ \hline \alpha A_1^T + \beta A_2^T & C \end{array}\right] \quad Q = \left[\begin{array}{c|c} \hat{Q} & \frac{a}{2}A_1 + \frac{b}{4}A_2 + \frac{c}{6}A_3 \\ \hline -\frac{a}{2}A_1^T - \frac{b}{4}A_2^T - \frac{c}{6}A_3^T & S \end{array}\right]$$

$$H = \left[\begin{array}{c|c} \hat{H} & yA_1 + xA_2 \\ \hline yA_1^T + xA_2^T & D \end{array}\right]$$

Now we wish to find a matrix H such that HP is symmetric, and HQ satisfies (17), if both of these conditions hold then our scheme satisfies the summation by parts conditions. We write $W = HP$ and $V = HQ$, then:

$$W = \left[\begin{array}{c|c} \hat{H}\hat{P} + (yA_1 + xA_2)(\alpha A_1^T + \beta A_2^T) & \alpha \hat{H} A_1 + \beta \hat{H} A_2 + yA_1 C + xA_2 C \\ \hline yA_1^T \hat{P} + xA_2^T \hat{P} + \alpha D A_1^T + \beta D A_2^T & (yA_1^T + xA_2^T)(\alpha A_1 + \beta A_2) + DC \end{array}\right] \tag{42}$$

$$V = \left[\begin{array}{c|c} \hat{H}\hat{Q} - (yA_1 + xA_2)(\frac{a}{2}A_1^T + \frac{b}{4}A_2^T + \frac{c}{6}A_3^T) & \frac{a}{2}\hat{H}A_1 + \frac{b}{4}\hat{H}A_2 + \frac{c}{6}\hat{H}A_3 + yA_1 S + xA_2 S \\ \hline yA_1^T\hat{Q} + xA_2^T\hat{Q} - \frac{a}{2}DA_1^T - \frac{b}{4}DA_2^T - \frac{c}{6}DA_3^T & (yA_1^T + xA_2^T)(\frac{a}{2}A_1 + \frac{b}{4}A_2 + \frac{c}{6}A_3) + DS \end{array}\right] \tag{43}$$

Now we take the symmetry conditions on W and V, first considering $W_1 = \hat{H}\hat{P} + (yA_1 + xA_2)(\alpha A_1^T + \beta A_2^T)$. In order for W to be symmetric we need W_1 to be symmetric.

Since $(yA_1 + xA_2)(\alpha A_1^T + \beta A_2^T)$ is automatically symmetric. This leaves the condition:

$$\hat{H}\hat{P} = (\hat{H}\hat{P})^T. \tag{44}$$

We also require that $V_1 = \hat{H}\hat{Q} - (yA_1 + xA_2)(\frac{a}{2}A_1^T + \frac{b}{4}A_2^T + \frac{c}{6}A_3^T) = \lambda\delta_{0,0}I$. Rearranging gives the condition:

$$\hat{H}\hat{Q} + (\hat{H}\hat{Q})^T = \begin{bmatrix} \lambda & \cdots & \cdots & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & (-\frac{c}{6}x) & (-\frac{c}{6}y) \\ 0 & \cdots & (-\frac{c}{6}x) & (-\frac{b}{2}x) & (-\frac{a}{2}x - \frac{b}{4}y - \frac{c}{6}x) \\ 0 & \cdots & (-\frac{c}{6}y) & (-\frac{a}{2}x - \frac{b}{4}y - \frac{c}{6}x) & (-ay - \frac{b}{2}x) \end{bmatrix} \tag{45}$$

The conditions on $W_4 = (yA_1^T + xA_2^T)(\alpha A_1 + \beta A_2) + DC$ and $V_4 = (yA_1^T + xA_2^T)(\frac{a}{2}A_1 + \frac{b}{4}A_2 + \frac{c}{6}A_3) + DS$ are automatically satisfied, by the forms of the matrices. Finally we have the two conditions $W_2 = W_3^T$ and $V_2 = -V_3^T$.

Expanding $W_2 = W_3^T$ gives:

$$\alpha h_{k,n} + \beta h_{k,n-1} = \begin{cases} xp_{n-1,k} + yp_{n,k} & \text{if } k \le n-2 \\ xp_{n-1,n-1} + yp_{n,n-1} - x + \beta z & \text{if } k = n-1 \\ xp_{n-1,n} + yp_{n,n} - \alpha x + (\beta - 1)y + \alpha z & \text{if } k = n \end{cases} \tag{46}$$

$$\beta h_{k,n} = \begin{cases} xp_{n,k} & \text{if } k \le n-2 \\ xp_{n,n-1} - \alpha x + \beta y & \text{if } k = n-1 \\ xp_{n,n} - x + \beta z & \text{if } k = n \end{cases} \tag{47}$$

Combining those together and assuming $\beta \neq 0$ transforms (46) into:

$$\beta h_{k,n-1} = \begin{cases} xp_{n-1,k} + yp_{n,k} - \frac{\alpha}{\beta}xp_{n,k} & \text{if } k \le n-2 \\ xp_{n-1,n-1} + yp_{n,n-1} - \frac{\alpha}{\beta}xp_{n,k} + (\frac{\alpha^2}{\beta} - 1)x - \alpha y + \beta z & \text{if } k = n-1 \\ xp_{n-1,n} + yp_{n,n} - \alpha h_{k,n} + \alpha(\frac{1}{\beta} - 1)x + (\beta - 1)y & \text{if } k = n \end{cases} \tag{48}$$

Expanding $V_2 = -V_3^T$ gives:

$$\frac{a}{2}h_{k,n} + \frac{b}{4}h_{k,n-1} + \frac{c}{6}h_{k,n-2} = \begin{cases} -xq_{n-1,k} - yq_{n,k} & \text{if } k \leq n-3 \\ -xq_{n-1,n-2} - yq_{n,n-2} + \frac{c}{6}z & \text{if } k = n-2 \\ -xq_{n-1,n-1} - yq_{n,n-1} + \frac{c}{6}y + \frac{b}{4}z & \text{if } k = n-1 \\ -xq_{n-1,n} - yq_{n,n} + \frac{a}{2}x + \frac{c}{6}x + \frac{b}{4}y + \frac{a}{2}z & \text{if } k = n \end{cases} \tag{49}$$

$$\frac{b}{4}h_{k,n} + \frac{c}{6}h_{k,n-1} = \begin{cases} -xq_{n,k} & \text{if } k \leq n-3 \\ -xq_{n,n-2} + \frac{c}{6}y & \text{if } k = n-2 \\ -xq_{n,n-1} - \frac{a}{2}x + \frac{b}{4}y + \frac{c}{6}z & \text{if } k = n-1 \\ -xq_{n,n} + \frac{c}{6}y + \frac{b}{4}z & \text{if } k = n \end{cases} \tag{50}$$

$$\frac{c}{6}h_{k,n} = \begin{cases} 0 & \text{if } k \leq n-3 \\ \frac{c}{6}x & \text{if } k = n-2 \\ \frac{c}{6}y & \text{if } k = n-1 \\ \frac{c}{6}z & \text{if } k = n \end{cases} \tag{51}$$

For $k = 0, .., n$ where $n+1$ is the size of the boundary block (because we are indexing from 0). We can simplify by assuming none of our constants are equal to 0, and substituting (50) into (51) and then into (49). We can then equate equations for $h_{k,j}$ to derive expressions relating the elements of $\hat{P}$ to $\hat{Q}$.

We can derive another relationship between $\hat{P}$ and $\hat{Q}$ by considering the necessary accuracy condition at the boundary. For stability, it has been shown that an $(n+1)th$ order scheme needs only to be nth order accurate at the boundary [5, 14]. Therefore to create a 6th order accurate scheme we only require 5th order accuracy in the boundary. To reach 5th order accuracy we require that substitutions of the equations $u_j = j^r$ and $\frac{du}{dj} = rj^{r-1}$ into Q and P respectively are exactly solved, where r is less than or equal to the order of accuracy desired. For our matrices we have:

$$
\begin{aligned}
r\sum_{j=0}^{n} p_{k,j} j^{r-1} &+ r\delta_{k,n-1}\beta(n+1)^{r-1} + r\delta_{k,n}\left[\alpha(n+1)^{r-1} + \beta(n+2)^{r-1}\right] \\
&= \sum_{j=0}^{n} q_{k,j} j^{r} + \frac{c}{6}\delta_{k,n-2}(n+1)^r + \delta_{k,n-1}\left[\frac{b}{4}(n+1)^r + \frac{c}{6}(n+2)^r\right] \\
&\qquad + \delta_{k,n}\left[\frac{a}{2}(n+1)^r + \frac{b}{4}(n+2)^r + \frac{c}{6}(n+3)^r\right] \\
&\qquad\qquad k = 0, ..., n \text{ and } r = 0, ..., r_0 \qquad (52)
\end{aligned}
$$

Where r_0 is the required order of accuracy. For our 6th order scheme, $r_0 = 5$, to retain this accuracy, we require $n \geq 5$ [14]. We now write this set of relations in matrix form. We let:

$$
T = \begin{bmatrix}
0\times 0^{-1} & 1\times 0^0 & 2\times 0^1 & 3\times 0^2 & 4\times 0^3 & 5\times 0^4 \\
0\times 1^{-1} & 1\times 1^0 & 2\times 1^1 & 3\times 1^2 & 4\times 1^3 & 5\times 1^4 \\
0\times 2^{-1} & 1\times 2^0 & 2\times 2^1 & 2\times 2^2 & 4\times 2^3 & 5\times 2^4 \\
0\times 3^{-1} & 1\times 3^0 & 2\times 3^1 & 3\times 3^2 & 4\times 3^3 & 4\times 4^4 \\
0\times 4^{-1} & 1\times 4^0 & 2\times 4^1 & 3\times 4^2 & 4\times 4^3 & 5\times 4^4 \\
0\times 5^{-1} & 1\times 5^0 & 2\times 5^1 & 3\times 5^2 & 4\times 5^3 & 5\times 5^4
\end{bmatrix}
$$

$$
M = \begin{bmatrix}
0^0 & 0^1 & 0^2 & 0^3 & 0^4 & 0^5 \\
1^0 & 1^1 & 1^2 & 1^3 & 1^4 & 1^5 \\
2^0 & 2^1 & 2^2 & 2^3 & 2^4 & 2^5 \\
3^0 & 3^1 & 3^2 & 3^3 & 4^4 & 3^5 \\
4^0 & 4^1 & 4^2 & 4^3 & 4^4 & 4^5 \\
5^0 & 5^1 & 5^2 & 5^3 & 5^4 & 5^5
\end{bmatrix}
\qquad
G = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
c_{3,0} & c_{3,1} & c_{3,2} & c_{3,3} & c_{3,4} & c_{3,5} \\
c_{4,0} & c_{4,1} & c_{4,2} & c_{4,3} & c_{4,4} & c_{4,5} \\
c_{5,0} & c_{5,1} & c_{5,2} & c_{5,3} & c_{5,4} & c_{5,5}
\end{bmatrix}
$$

So we have:

$$
\hat{P}T = \hat{Q}M + G \qquad (53)
$$

Where the constants $c_{i,j}$ are functions of α, β, a, b and c, we can use (36) - (38) to write these in terms of just two of the variables, and as soon as we fix two of these parameters we will just have constants. We interpret 0×0^{-1} as 0 and $0^0 = 1$ since they are derived by differentiating $f(x) = 1$ to get $f'(x) = 0$. With this in mind we see that neither matrix is singular so we can easily rearrange this expression to get $\hat{Q}$ in terms of $\hat{P}$. Using MATLAB [15] we use this to rewrite equations (49) - (51) in terms of the elements of $\hat{P}$ which gives us expressions for the last three columns of $\hat{H}$ in terms of the last two rows of $\hat{P}$. We then equate these equations with (47) and (48) giving us a linear system in the elements of the last two rows of $\hat{P}$ in terms of $x, y, z, \alpha, \beta, a$ and b which we can solve in MATLAB. We can then simplify this by using (36) - (38) to remove some of the variables, before substituting this back in to (49), (50) and (51) to have expressions for the last two rows of $\hat{Q}$ and the last two columns of $\hat{H}$ in terms of just x, y, z and our remaining constants. These expressions are very long so have been omitted.

We now multiply (53) by $\hat{H}$ to get:

$$\hat{V} = \hat{W}TM^{-1} - \hat{H}GM^{-1} \tag{54}$$

where $\hat{W} = \hat{H}\hat{P}$ and $\hat{V} = \hat{H}\hat{Q}$. The form of G means that the only contributions from $\hat{H}$ in the right most term come from the three columns of $\hat{H}$ that we already know in terms of x, y, z and our constants. We can combine (54) with the symmetry conditions (44) and (45) to get an equation we hope to be able to solve for $\hat{W}$ and $\hat{V}$ which will give us a nonlinear systems of equations for $\hat{P}$, $\hat{Q}$ and $\hat{H}$ which we can solve using numerical and computational methods. Taking $\hat{W}$ to be symmetric, such that:

$$\hat{W} = \begin{bmatrix} w_{0,0} & \dots & w_{0,5} \\ \vdots & \ddots & \vdots \\ w_{0,5} & \dots & w_{5,5} \end{bmatrix}$$

Then we require:

$$\begin{aligned} \hat{V} + \hat{V}^T &= \hat{W}TM^{-1} - \hat{H}GM^{-1} + (TM^{-1})^T\hat{W} - (GM^{-1})^T\hat{H}^T \\ &= \begin{bmatrix} \lambda & \cdots & \cdots & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & (-\frac{c}{6}x) & (-\frac{c}{6}y) \\ 0 & \cdots & (-\frac{c}{6}x) & (-\frac{b}{2}x) & (-\frac{a}{2}x - \frac{b}{4}y - \frac{c}{6}x) \\ 0 & \cdots & (-\frac{c}{6}y) & (-\frac{a}{2}x - \frac{b}{4}y - \frac{c}{6}x) & (-ay - \frac{b}{2}x) \end{bmatrix} \end{aligned} \tag{55}$$

This is a system of linear equations in the elements of $\hat{W}$. Using MATLAB we find that in general this system has no solutions since the system contains 36 equations which in general are linearly independent, but only 21 unknowns due to the symmetry of $\hat{W}$, so this system has no solutions.

B. Tridiagonal, 6th Order, 7 Point implicit SBP Schemes

Following the previous section, if we instead take the special case where $\beta = 0$, and let $n = 5$, equations (46), (47) and (52) are simplified into:

$$\alpha h_{k,5} = \begin{cases} xp_{4,k} + yp_{5,k} & \text{if } k \leq 3 \\ xp_{4,4} + yp_{5,4} - x & \text{if } k = 4 \\ xp_{4,5} + yp_{5,5} - \alpha x - y + \alpha z & \text{if } k = 5 \end{cases} \tag{56}$$

$$0 = \begin{cases} xp_{5,k} & \text{if } k \leq 3 \\ xp_{5,4} - \alpha x & \text{if } k = 4 \\ xp_{5,5} - x & \text{if } k = 5 \end{cases} \tag{57}$$

$$\begin{aligned} r\sum_{j=0}^{5} p_{k,j} j^{r-1} &+ r\delta_{k,5}\alpha(6)^{r-1} \\ &= \sum_{j=0}^{5} q_{k,j} j^r + \frac{c}{6}\delta_{k,3}(6)^r + \delta_{k,4}\left[\frac{b}{4}(6)^r + \frac{c}{6}(7)^r\right] \\ &\quad + \delta_{k,5}\left[\frac{a}{2}(6)^r + \frac{b}{4}(7)^r + \frac{c}{6}(8)^r\right] \\ &\qquad k = 0, ..., n \text{ and } r = 0, ..., r_0 \end{aligned} \tag{58}$$

This can be written in matrix form analogous to (53). Additionally, we now only have one degree of freedom between our constants so we can use (36) - (38) to write a, b and c in terms of α.

We can immediately solve (57) to get:

$$p_{5,k} = \begin{cases} 0, & \text{if } k \leq 3 \\ \alpha, & \text{if } k = 4 \\ 1, & \text{if } k = 5 \end{cases} \tag{59}$$

Which also matches our interior scheme. Substituting this into (56) and assuming $\alpha \neq 0$ gives us:

$$h_{k,5} = \begin{cases} \frac{x}{\alpha} p_{4,k} & \text{if } k \leq 3 \\ \frac{x}{\alpha} p_{4,4} - \frac{x}{\alpha} + y & \text{if } k = 4 \\ \frac{x}{\alpha} p_{4,5} - x + z & \text{if } k = 5 \end{cases} \tag{60}$$

Similarly, from (51) we have:

$$h_{k,5} = \begin{cases} 0 & \text{if } k \leq 2 \\ x & \text{if } k = 3 \\ y & \text{if } k = 4 \\ z & \text{if } k = 5 \end{cases} \tag{61}$$

and substituting into (49) and (50) gives:

$$\frac{c}{6} h_{k,4} = \begin{cases} -xq_{5,k} & \text{if } k \leq 2 \\ -xq_{5,3} + \frac{c}{6}y - \frac{b}{4}x & \text{if } k = 3 \\ -xq_{5,4} - \frac{a}{2}x + \frac{c}{6}z & \text{if } k = 4 \\ -xq_{5,5} + \frac{c}{6}y & \text{if } k = 5 \end{cases} \tag{62}$$

$$\frac{c}{6} h_{k,3} = \begin{cases} -xq_{4,k} - yq_{5,k} + \frac{3b}{2c}xq_{5,k} + & \text{if } k \leq 2 \\ -xq_{4,5} - yq_{5,3} + \frac{c}{6}z - \frac{a}{2}x - \frac{3b}{2c}(-xq_{5,3} + \frac{c}{6}y - \frac{b}{4}x) & \text{if } k = 3 \\ -xq_{4,4} - yq_{5,4} + \frac{c}{6}y + \frac{b}{4}z - \frac{a}{2}y - \frac{3b}{2c}(-xq_{5,4} - \frac{a}{2}x + \frac{c}{6}z) & \text{if } k = 4 \\ -xq_{4,5} - yq_{5,5} + \frac{a}{2}x + \frac{c}{6}x + \frac{b}{4}y - \frac{3b}{2c}(-xq_{5,5} + \frac{c}{6}y) & \text{if } k = 5 \end{cases} \tag{63}$$

$$\tag{64}$$

Combining (60) and (61) we write:

$$p_{4,k} = \begin{cases} 0 & \text{if } k \leq 2 \\ \alpha & \text{if } k = 3 \\ 1 & \text{if } k = 4 \\ \alpha & \text{if } k = 5 \end{cases} \tag{65}$$

Which matches our interior scheme. Then taking (58) and using MATLAB we can write the last two rows of $\hat{Q}$ in terms of the last two rows of $\hat{P}$, and therefore, in terms of α.

$$q_{4,0} = \frac{-1031\alpha - 3}{10}, \qquad q_{4,1} = \frac{30869\alpha + 107}{60}, \qquad q_{4,2} = \frac{-20524\alpha - 87}{20},$$
$$q_{4,3} = \frac{4081\alpha + 21}{4}, \qquad q_{4,4} = -\frac{-3029\alpha - 27}{3}, \qquad q_{4,5} = \frac{1957\alpha + 51}{20}.$$

$$q_{5,0} = \frac{393\alpha - 6322}{130}, \qquad q_{5,1} = \frac{15832\alpha - 1141}{30}, \qquad q_{5,2} = \frac{5439\alpha - 63473}{60},$$
$$q_{5,3} = \frac{-6732\alpha + 63679}{60}, \qquad q_{5,4} = \frac{862\alpha - 6403}{12}, \qquad q_{5,5} = \frac{-549\alpha + 3206}{30}.$$

These values for $q_{4,k}$ and $q_{5,k}$ can then be substituted back into (62) - (63) which we then use together with (61) to solve the last three columns of $\hat{H}$ in terms of just α, x, y and z. The general form of $\hat{H}$ involves fairly long equations in α so has been omitted.

$$\hat{H}(\alpha = 1) = \begin{bmatrix} h_{0,0} & \cdots & h_{0,2} & -\frac{421509x}{4} - \frac{5929y}{2} & -\frac{5929x}{2} & 0 \\ \vdots & \ddots & \vdots & \frac{1044655x}{2} + 14691y & 14691x & 0 \\ \vdots & \ddots & \vdots & -1032003x - 29017y & -29017x & 0 \\ \vdots & \ddots & \vdots & 1014270x + 28508y + z & 28508x + y & x \\ \vdots & \ddots & \vdots & -\frac{1975663x}{4} - \frac{27745y}{2} & z - \frac{27747x}{2} & y \\ h_{5,0} & \cdots & h_{5,2} & \frac{189401x}{2} + 2657y & 2657x + y & z \end{bmatrix} \tag{66}$$

Going back to

$$\hat{V} = \hat{W}TM^{-1} - \hat{H}GM^{-1}$$

with $\hat{W}$ symmetric and $\hat{V} + \hat{V}^T$ almost asymmetric, we have that $\hat{W}TM^{-1} - \hat{H}GM^{-1}+$ derive a system of equations in the elements of $\hat{W}$.

$$\hat{V} + \hat{V}^T = \hat{W}TM^{-1} - \hat{H}GM^{-1} + (TM^{-1})^T\hat{W} - (GM^{-1})^T\hat{H}^T$$
$$= \begin{bmatrix} \lambda & \cdots & \cdots & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & (-\frac{c}{6}x) & (-\frac{c}{6}y) \\ 0 & \cdots & (-\frac{c}{6}x) & (-\frac{b}{2}x) & (-\frac{a}{2}x - \frac{b}{4}y - \frac{c}{6}x) \\ 0 & \cdots & (-\frac{c}{6}y) & (-\frac{a}{2}x - \frac{b}{4}y - \frac{c}{6}x) & (-ay - \frac{b}{2}x) \end{bmatrix}$$

With $\beta = 0$, we find that the resulting system is now symmetric giving us 21 equations to solve for our 21 unknowns. Using MATLAB we convert the system of equations into the form $K\mathbf{w} = \mathbf{x}(x, y, z, \alpha, \lambda)$, where K is the (21×21) matrix of coefficients of $w_{i,j}$ in each equation from the system and $\mathbf{x}$ is a (21×1) vector consisting of the elements of $\hat{W}$ which we wish to solve for. We compute the rank of our system (note that in doing this we assume that none of our constants equal 0) and find it to be 18 meaning our system is overdetermined and we will either have infinitely many, or no solutions. From linear algebra, we know that for there to be infinitely many solutions we require that $\text{rank}(K) = \text{rank}([K|\mathbf{x}])$; in general, $\text{rank}([K|\mathbf{x}]) = 19$ so we now look to find specific values of $x, y, z, \alpha,$ and λ such that the rank is only 18. We perform Gaussian elimination on K to put it into row reduced form, keeping track of the row operations used to do this. Then we apply the same row operations to $\mathbf{x}$. Since the row reduced form of K had three zero rows, we require that the bottom three rows of $\mathbf{x}$ after the same operations are applied are also zero. In doing this we make the assumption that none of our constants are equal to zero. This gives the following system:

$$\lambda - \frac{54x}{5} - 9y + z + \frac{517\alpha x}{5} + 29\alpha y - 3\alpha z = 0$$
$$\frac{241x}{30} + \frac{11y}{2} + \frac{3z}{5} - \frac{2363\alpha x}{30} - \frac{64\alpha y}{3} + \frac{\alpha z}{5} = 0$$
$$\frac{809\alpha x}{30} - \frac{11y}{6} - \frac{3z}{5} - \frac{13x}{5} + \frac{59\alpha y}{6} + \frac{23\alpha z}{10} = 0$$

We solve this for y, z, λ in terms of x and α:

$$y = -\frac{x(55967\alpha^2 - 15023\alpha + 978)}{5(3062\alpha^2 - 1195\alpha + 132)} \qquad z = \frac{x(35865\alpha^2 - 3531\alpha + 77)}{9186\alpha^2 - 3585\alpha + 396} \tag{67}$$

$$\lambda = \frac{x(657942\alpha^3 - 700911\alpha^2 + 111195\alpha - 5407)}{15(3062\alpha^2 - 1195\alpha + 132)} \tag{68}$$

Substituting these back into (54) now gives a linear system of equations with infinitely many solutions. We find one such solution and we see that x (as well as α) is left as a free parameter (we have rounded to two significant figures to fit on the page):

$$\hat{W}(\alpha = 1) = \begin{bmatrix} 8.8\times10^3x & -5.6\times10^4x & 3.5\times10^5x & 2.6\times10^5x & -1.2\times10^4x & -3.6x \\ -5.6\times10^4x & 3.4\times10^5x & -1.9\times10^6x & -8.2\times10^5x & 2.6\times10^5x & -51.0x \\ 3.5\times10^5x & -1.9\times10^6x & 6.5\times10^6x & -1.9\times10^6x & 3.7\times10^5x & -5.2\times10^3x \\ 2.6\times10^5x & -8.2\times10^5x & -1.9\times10^6x & 3.4\times10^5x & -5.5\times10^4x & 0 \\ -1.2\times10^4x & 2.6\times10^5x & 3.7\times10^5x & -5.5\times10^4x & 8.7\times10^3x & 0 \\ -3.6x & -51.0x & -5.2\times10^3x & 0 & 0 & 0 \end{bmatrix} \tag{69}$$

From this we can easily derive:

$$\hat{V}(\alpha = 1) = \begin{bmatrix} 1.0x & -6.2\times10^3x & -5.3\times10^5x & 5.4\times10^5x & 3.0\times10^3x & 488.0x \\ 6.2\times10^3x & 0 & 2.7\times10^6x & -3.3\times10^6x & 5.5\times10^5x & -3.9\times10^3x \\ 5.3\times10^5x & -2.7\times10^6x & 0 & 2.7\times10^6x & -5.3\times10^5x & 1.4\times10^3x \\ -5.4\times10^5x & 3.3\times10^6x & -2.7\times10^6x & 0 & -1.9\times10^4x & 1.7\times10^3x \\ -3.0\times10^3x & -5.5\times10^5x & 5.3\times10^5x & 1.9\times10^4x & -1.1x & 599.0x \\ -488.0x & 3.9\times10^3x & -1.4\times10^3x & -1.7\times10^3x & -599.0x & -4.1x \end{bmatrix} \tag{70}$$

We now have non-linear equations for $\hat{P}$, $\hat{Q}$ and $\hat{H}$. Furthermore, as the scheme contains some free parameters, α and x it should be possible to optimize the scheme further in a DRP like manner by choosing some error quanitifier to minimise. However, non-linear system must first be solved, this is likely best done computationally using a nonlinear solver and solving $\hat{H}\hat{P} = \hat{W}$ subject to the conditions (59) - (65), and then using (53) to find $\hat{Q}$. Attempting to solve this using MATLAB's *fsolve* non linear solver, and the interior scheme as our initial starting point unfortunately did not yield a close solution within 10000 function evaluations. Attempts were also made using variants of vectors made up of zeroes and ones as the starting point which were also in vain, therefore with the tools available, it was not possible to confirm whether the non linear system had solutions, nor test the performance of this new scheme against others. A more powerful non linear solver may be able to help with this stage.

Should a solution be found, since the scheme satisfies SBP properties, we would be able to impose any boundary conditions posed by a problem using SATs, it should also be relatively simple to optimise over the dispersion relation in a fashion similar to in [10]. The method for doing this would be to apply the scheme to a specific test function with a known derivative, for example, a plane wave or an exponentially growing wave. Then one could computationally find the dispersion error as determined by whichever metric we have chosen and minimise this with respect to the free parameters. Then we would use those parameters in our scheme for use on other, similar problems in the hope that they would minimise the dispersion error in those too. Unfortunately, due to the lack of explicit solution for P, Q and H this remains to be done for this specific scheme.

IV. Conclusions

In the theory section of this report we described and outlined the current theory behind finite difference schemes and the criteria required for them to be of a given order on the interior of the scheme. We then considered both DRP and SBP schemes and analysed the advantages and disadvantages of each. We concluded that for acoustical problems, it is beneficial to use DRP schemes as generally they better represent the physics of waves. From understanding how DRP schemes are optimized we were able to ensure that we would have free parameters available when constructing our scheme which would enable us to create a physically accurate scheme for wave equations.

We also summarised the current theory behind SBP schemes and applied it to the example case of the 1D advection equation. The stability that the SBP property imposes is of huge relevance to acoustics problems where we frequently encounter phenomena such as shocks and blow ups, deciding to enforce SBP properties on our scheme ensures that it will be stable. Additionally, creating an SBP scheme allows us to later impose SATs to our scheme enabling it to be applied to problems other than simple homogeneous ones. This is useful for acoustical problems where the physical model is often complex and it is convenient to have a versatile scheme which can be adapted for use in many situations. Furthermore, constructing an implicit scheme would allow us to use fewer points per wavelength in our approximation without sacrificing global accuracy which is a useful trait in modelling waves.

Through literature review we realised that a finite difference scheme with all of the above properties did not exist above fourth order accuracy. In the results section, we outlined a systematic method for finding a sixth order scheme. We found that using a 7 point stencil was optimal due to the simple form it gave us for our matrices. We chose this over a 5 point stencil as the additional equations in (51) enabled us to solve our conditions so that our $\hat{P}$ matrix matched the interior scheme for the last two rows. This also gave us an extra coefficient which could later be used to optimize the scheme in a DRP like fashion and so our scheme could meet all of the criteria outlined above.

Through computational approaches we showed that such a scheme could only exist if it were tridiagonal, taking this specific case we then systematically approached solving the criteria for the scheme. We were able to derive an implicit form of the scheme which still left two free variables which could be used for DRP optimization. Unfortunately, we were left with a 36 dimensional non-linear system of equations in 48 variables which is yet to be solved.

The next steps in this research area would be to design an algorithm which could solve this system allowing us to express $\hat{P}$, $\hat{Q}$ and $\hat{H}$ explicitly, once this had been done we could vary the values of α and x, our free parameters, and optimize in a DRP like fashion, such that the physics of the wave solution are preserved, then all that would remain would be to test the performance of this scheme relative to other schemes. This could be done by selecting a test function on which to compare performance, and considering an error metric relevant to the problem which would likely include measuring dispersion error. The degrees of freedom mean we can easily modify any solutions of the non-linear system to suit particular problems where certain errors are more important to avoid than others.

Beyond this, further research could include constructing higher order schemes. This could be done by following the methodology in this report and making adjustments to the matrices involved in deriving the criteria to solve for. Since the approach used was very systematic it could be possible for a computer to generate schemes of much higher orders of accuracy. The limiting factor of the current approach remains the difficulty of solving the non-linear system reached (though this was done for fourth order in [14]), with increased time and computing power this problem could hopefully be surpassed. One possibility could be to use a large enough boundary block that we could remove some of the non-linearity by fixing many of the coefficients in the $\hat{P}$ matrix, however this would require a large boundary block which may not be appropriate for specific problems.

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