PX402 Interim Report - Making Waves with Finite Differences

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I. Motivation

Computational aeroacoustics (CAA) is an area of interest as developments can lead to better control of noise levels from vehicles, simulating sound propagation etc. Modern computers have facilitated the direct computational simulation of acoustical problems which is a powerful tool with many potential applications including engineering quieter vehicles, simulating sound propagation into the atmosphere and designing musical instruments. To computational 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 phenomena such as shocks and blow ups. Currently a lot of effort is being put into developing finite difference schemes for derivatives in ways that ensure the physics of the wave propagation are preserved [1]. Many physical properties depend on the dispersion relation of the wave, conventional finite difference schemes are often poor at preserving these properties. However, Dispersion Relation Preserving 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 [2, 3].

Another class of schemes known as Summation by Parts (SBP) schemes have been show to be both well-posed and provably stable [1] as they exhibit a property similar to integration by parts. This property allow us to weakly impose boundary conditions by using the method of Simultaneous Approximation Terms (SATs) [4].

The aim of this project is to investigate the strengths and weaknesses of the two kinds of finite difference scheme and attempt to develop and combine the techniques, in various ways. We then hope to use the results of these investigations to construct new schemes with various properties and orders, and compare their performance to existing schemes. We hope to be able to prove or disprove whether it is possible to have higher order schemes which simultaneously hold both DRP and SBP properties and also look into new methods for optimizing existing schemes.

II. Theory

A. Preliminaries and Notation

Let our domain be split into a grid with $n+1$ equally spaced grid points indexed from 0 to n. Derivatives are approximated by linear combinations of the function values at grid points. 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 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:

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

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

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

Where H and Q are $(n+1)\times(n+1)$ matrices and $\mathbf{u}$ and $\mathbf{u}'$ are $n+1$ dimensional vectors representing the function and its derivative at each grid point. The relations between the coefficients a_j and β_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 [2], are known as Maximal Order (MO) schemes. The relations up to 10th order are detailed in (2.1.1)-(2.1.5) of [5]. 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 (β_j) terms to simplify the computation, for example, in a 7-point, 4th order family of schemes, we have three parameters so that:

$$a_2(u'_{i-2} + u'_{i+2}) + a_1(u'_{i-1} + u'_{i+1}) + u'_i = \beta_3 \frac{u_{i+3} - u_{i-3}}{6\Delta x} + \beta_2 \frac{u_{i+2} - u_{i-2}}{4\Delta x} + \beta_1 \frac{u_{i+1} - u_{i-1}}{2\Delta x}$$

and we must also satisfy two relations between the coefficients to reach 4th order accuracy [5]. We can set $a_2 = 0$ to generate 3-point diagonal schemes, the accuracy relations leave three parameters, or degrees of freedom, spare. If we were to require 6th order accuracy, the increase in relations would leave us with only two degrees of freedom. We could also set $\beta_3 = 0$ which would give us 4th order, 3-point diagonal schemes with one degree of freedom. Likewise, if we set $a_1 = a_2 = 0$ we would have an explicit (1-point diagonal) scheme for u'_i but only one degree of freedom.

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.

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. We can do this by utilizing the property that the wave number of a derivative is proportional to the wave number of the original function [5, 6]. 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. Taking the Fourier transform of both sides of (2) with $a_j = 0 \; \forall j$, and dividing through by $\tilde{u}$ we get that the wave number of the finite difference scheme $\bar{\alpha}$ satisfies:

$$i\bar{\alpha} = \frac{1}{\Delta x} \sum_{j=1}^{\frac{n-1}{2}} \beta_j e^{i\alpha j \Delta x}$$

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 [6] used this error quantity:

$$E = \int_{\frac{-\pi}{2}}^{\frac{\pi}{2}} |i\kappa - \sum_{j=1}^{\frac{n-1}{2}} \beta_j e^{ij\kappa}|^2 dk$$

$$\text{with } \kappa = \alpha \Delta x$$

While Maximal Order schemes have low truncation errors, they often do poorly at minimising the dispersion error. Dispersion Relation Preserving (DRP) schemes, initially proposed by Tam and Webb in [6], 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 E with respect to the spare coefficients. Such schemes require fewer points per wavelength to accurately resolve constant amplitude waves [3]. 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.

C. Exponential Wave Functions

For a constant amplitude plane wave of the form $u(x) = \Re(Ae^{i\alpha x}) = Acos(\alpha x)$ with derivative $u'(x) = \Re(i\alpha Ae^{i\alpha x})$ the finite difference scheme gives us an approximation $\bar{\alpha}$ for the wave number α.

Using (2), and setting $a_j = 0$ for all j to give an explicit scheme and relabelling the index we have:

$$u'_k \approx \frac{1}{\Delta x} \sum_{j=1}^{\frac{n-1}{2}} \beta_j \left(u_{k+j} - u_{k-j}\right) \tag{4}$$

Now we see that our approximation:

$$u'_k \approx \Re\left(\frac{Ae^{i\alpha kx}}{\Delta x} \sum_{j=1}^{\frac{n-1}{2}} \beta_j \left(e^{i\alpha j\Delta x} - e^{-i\alpha j\Delta x}\right)\right) = \Re\left(\frac{2iAe^{i\alpha kx}}{\Delta x} \sum_{j=1}^{\frac{n-1}{2}} \beta_j sin(\alpha j \Delta x)\right)$$

Taking the left hand side $u'_k = \Re(i\bar{\alpha}Ae^{i\bar{\alpha}kx})$ we get

$$\bar{\alpha}\Delta x = 2\sum_{j=1}^{\frac{n-1}{2}} \beta_j sin(\alpha j\Delta x).$$

After matching L terms to the Taylor we then optimize using our degrees of freedom so that $\bar{\alpha}$ is close as possible to α. Using (2) we derive:

$$\bar{\alpha}\Delta x = \frac{2\sum_{j=1}^{\frac{n-1}{2}} \beta_j sin(\alpha j\Delta x)}{1+2\sum_{j=1}^{M} a_j cos(\alpha j\Delta x)}. \, [3] \tag{5}$$

The value of M determines the "diagonality" of the scheme. When α is complex (for exponentially growing or decaying waves), it has been shown that MO schemes do better than DRP schemes at optimizing $\bar{\alpha}$ despite the fact that DRP schemes have been designed for this purpose [3]. This is because DRP schemes are sensitive to the value of $arg(\alpha\Delta x)$ whereas MO schemes are not. This means for MO schemes the number of points per (complex) wavelength can just depend on the magnitude $|\alpha\Delta x|$ 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 [3] were not demonstrated until more recently.

D. Summation By Parts Schemes

Although higher order approximations give better truncation error tolerance and are best for time dependent problems where we need a high resolution, in practice for many types of problem, including many in acoustics, we don't need particularly high accuracy due to the fact there is a lot of physical error in the model anyway. 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) [7]. Our proof of the necessary properties for this upper bound to exist is based on an energy method [4].

Starting from the 1D advection equation (which we will use as our example problem), with some scalar field $u(x, t)$ with positive unit wave speed:

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0 \tag{6}$$

With $x_L \leq x \leq x_R$, $u(0,t) = u_L(t) = 0$ and $u_L = 0$ The rate of change of energy E with respect to time is:

$$\frac{dE}{dt} = -2\int_{x_L}^{x_R} u\frac{\partial u}{\partial x}dx$$

Applying integration by parts yields:

$$\frac{d}{dt}\int_{x_L}^{x_R} u^2 dx = -(u_R^2 - u_L^2) \tag{7}$$

Which is nonpositive when $u_L = 0$. Therefore, our problem is bounded and so with initial conditions is well posed [8].

Considering a discretisation in space such that $\boldsymbol{u} = [u_0, u_1, ...u_n]^T$ and letting D be an operator representing the first derivative we take:

$$HD\boldsymbol{u} = Q\boldsymbol{u} \tag{8}$$

We now want to find H and Q (if they exist) such that:

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

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

$$\langle \boldsymbol{u}, \boldsymbol{v}\rangle_H = \boldsymbol{u}^T H\boldsymbol{v} \tag{9}$$

$$||\boldsymbol{u}||^2 = \boldsymbol{u}^T H\boldsymbol{u} \tag{10}$$

$$\int_{x_L}^{x_R} uv dx \approx \boldsymbol{u}^T H\boldsymbol{v} = \langle \boldsymbol{u}, \boldsymbol{v}\rangle_H \tag{11}$$

and Q such that:

$$Q + Q^T = E_n - E_0 = diag[0, ..., 0, 1] - diag[1, 0, ..., 0] \tag{12}$$

Where E_i are matrices who have 1 as the ith value of their diagonal and are zero elsewhere. We see that when (9)-(12) hold, a property similar to integration by parts - known as summation by parts (SBP) - also holds. The integration by parts formula is:

$$\int_\Omega uv dx = uv|_\Omega - \int_\Omega v\frac{\partial u}{\partial x}dx \tag{13}$$

The discrete analog of this which (9)-(12) are necessary and sufficient for [5] is:

$$\langle \boldsymbol{u}, \boldsymbol{v}\rangle_H = \boldsymbol{u}^T(E_n - E_0)\boldsymbol{v} - \langle H^{-1}Q\boldsymbol{u}, \boldsymbol{v}\rangle \tag{14}$$

This implies that an approximation scheme with conditions (9)-(12) will yield the same energy estimate as the analytical approach, proving the approximation is time stable [4]:

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

The general method for constructing SBP schemes is to begin with a stencil and then make modifications at the grid points and boundaries to ensure (9)-(12) are satisfied along with the accuracy conditions. This process is well documented in [5] 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 [2, 1] schemes has been achieved. However this area od study remains fairly limited.

E. Simultaneous Approximation Terms

Simultaneous Approximation Terms (SATs) deal with the issues that arise at the boundaries however they rely on problem being well posed and stable [4] so are only applicable with stable schemes such as SBP schemes. They 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. Using the 1D advection equation as our example, we start from (8) but introduce an additional parameter σ:

$$HD\boldsymbol{u} = Q\boldsymbol{u} + \sigma(u_0 - u_L)\boldsymbol{e_0} \tag{15}$$

where $\boldsymbol{e_0} = (1, 0, ..., 0)^T$. We then calculate the same energy estimate as before and find:

$$\frac{d\boldsymbol{u}^T H\boldsymbol{u}}{dt} = -(u_n^2 - u_0^2) - 2\sigma u_0^2$$

Which is nonnegative for $\sigma \geq \frac{1}{2}$. We must also choose σ such that Gauss' Theorem holds for our discrete operators i.e.

$$\begin{aligned} (u_R - u_L) &= \int_{x_L}^{x_R} \frac{\partial u}{\partial x} dx & &\approx \langle \mathbf{1}, D\boldsymbol{u}\rangle_H \\ &= \mathbf{1}^T HD\boldsymbol{u} & &= \mathbf{1}^T Q\boldsymbol{u} + \mathbf{1}^T \sigma(u_0 - u_L)\boldsymbol{e_0} \\ &= (u_n - u_0) + \sigma(u_0 - u_L) & &\implies \sigma = 1 \end{aligned}$$

so we see that choosing $\sigma = 1$ choice ensures both conservation and stability [4, 8].

III. Term 1 Work Done

The focus of last term was largely on understanding the background theory of both DRP and SBP schemes. The first week or so of term was used to read general theory behind finite difference schemes and ensure I had a solid foundation there. I studied [6] and [9] which gave some overview as well as various online resources, books and lecture notes at undergraduate and graduate level including [10, 11, 12, 13]. I also read the first bits of [5] and derived accuracy relations for a second order scheme by hand to consolidate my understanding of the parameters, particularly the appearance of degrees of freedom which would become relevant to DRP schemes.

The next 2-3 weeks were spent learning the theory behind DRP schemes, including reading [3, 5, 6]. I went back to [9] which gave further insight into the advantages of the schemes. I wrote up a summary of my understanding and did many hand calculations to derive each of the equations for myself to aid in understanding. One point of difficulty I overcame was the inconsistency of notation between papers; it took a while to fully understand the terminology used and why certain combinations of coefficients had certain degrees of freedom. I used the example detailed by [5] extensively to aid my understanding and used the relations given to work out how the free parameters changed and why you could choose certain values for some orders of scheme. I also spent time understanding the problems with exponentially growing and decaying waves as noted in [3].

The next 3-4 weeks were similar but for SBP schemes and SATs. I mostly used [4] but also [1, 2, 14] and manually derived many of the calculations and proofs. I found looking at the examples of schemes given in [1, 2] helpful and was able to then derive a system of equations required to be satisfied, for a simple example. The example of implementing SATs in [2] also helped a lot with understanding these.

Throughout the process I spent time experimenting with schemes for simple equations, mainly the 1D advection equation. I derived equations using a very simple SBP scheme and looked at how this could be combined with a DRP scheme but had trouble when it came to the boundaries. Most of weeks 9 and 10 were spent experimenting and testing combinations of schemes but the approach I was taking ended up with very computationally demanding linear algebra which I was unable to complete. I struggled a little with not having a particular goal to work towards other than making a better scheme so it was very useful spending some time at the end of the term to assess the knowledge gained and define some clear objectives for research.

IV. Targets for Term 2

I've identified four main areas of possible research for term 2. Each develops known theory and adapts it to create new schemes which will aim to either deal with some of the aforementioned problems, or be of higher order/accuracy than current schemes. It is difficult to tell how long these tasks will take, I expect to achieve two of them within the time frame given. I will need to write or adapt code to compare any new schemes with existing schemes as well as to solve any derived systems of equations. The aim is to write up my work as I go and be ready to write the final report by week 8.

1. **Optimizing the degrees of freedom in the boundary blocks of a 4th order, 7-point DRP scheme.** Beginning with an existing fourth order scheme as the interior scheme. I will determine an asymmetric scheme to use near the boundaries and follow the approach in [15] (min. 1.5 weeks). The challenge will be optimizing boundary blocks whilst imposing boundary conditions and maintaining stability. I will write the problem down, choose an equation to solve and a metric to optimize over (min. 2 weeks), then derive a system of equations, find free variables and optimize. Finally, I will compare the results with existing schemes (min. 2 weeks including writing code).

2. **Construct a 4th order DRP scheme with a diagonal H matrix.** First I need to work out if this is possible, this will involve deriving a system of equations and doing some algebraic manipulation (min. 1.5 weeks). If it is possible, I will work out how many degrees of freedom there are and what size of stencil should be used. Then solve the system and compare the scheme to existing ones (min. 1 week).

3. **Construct 6th and/or 8th order tridiagonal, implicit SBP schemes (the highest order constructed to date is 4th order).** Start by writing down the necessary accuracy conditions. These will be combined with (9)-(12). I plan on following a similar method to Strand in [14]. (min. 3 weeks)

4. **Work out if it is possible to create a 7-point, tridiagonal, 6th order DRP, SBP scheme.** Following from task 3, I would investigate the possibility of deriving a system of equations with free parameters to optimize over. An explicit, 7 point, DRP, SBP scheme exists in [2] however it is only 4th order accurate. (This is the most difficult task and very hard to estimate a length of time for).

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