Making Waves with Finite Differences

Deriving Finite Difference Schemes for Computational Aeroacoustics

William Bolton - 1300316

Abstract

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.

Motivation

Computational aeroacoustics is an area of particular industrial interest as developments can lead to better simulation of sound propagation. 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:

Since computers are unable to exactly compute limits to zero, many discrete, finite difference approximation schemes exist to approximate derivatives computationally. In the realm of aeroacoustics, additional difficulties arise:

- 1. Ensuring the physics of the wave propagation, governed by the dispersion relation between wavenumber and frequency, are preserved.
- 2. Ensuring the approximation remains stable in the presence of singularities and discontinuities common in the realm of aeroacoustics due to phenomena such as shocks and blow up. We wish to construct a new finite difference scheme that deals with these problems.

Finite Difference Schemes

Finite Difference schemes model derivatives to functions by dividing the domain into a grid and manipulating truncated Taylor Series. We take linear combinations of the function values at local grid points and express them in terms of their Taylor series to approximate the derivative [6]. A few simple cases of this using the first term of the expansion are illustrated in Figure 1.

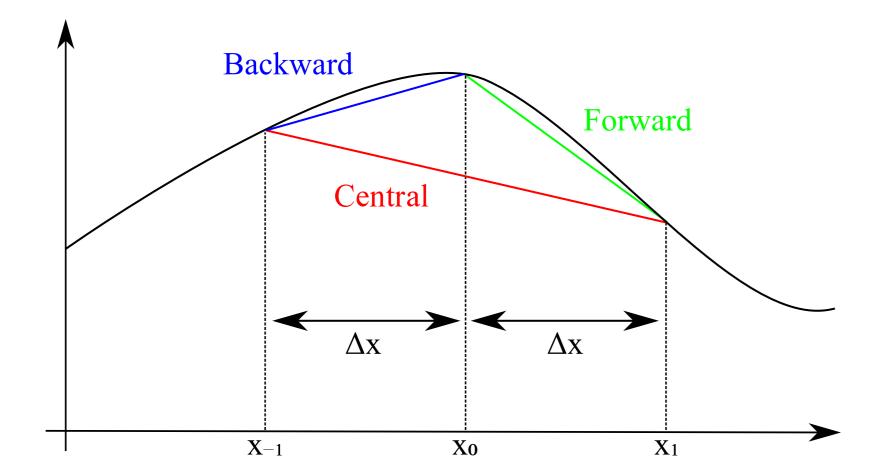


Figure 1: Simple first order finite difference schemes for the derivative of the curve at x_0 using a 3 point stencil.

By taking the series at further points and including higher order Taylor terms we can get higher order approximations. In general the definition of a central scheme defined on the interior of the domain, with an n point stencil which is 2M + 1 diagonal we have [3]:

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

Where u_i is the function value at the *ith* grid point, and u'_i is its approximate derivative. The relations between the coefficients β_i and a_i 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.

Schemes are called explicit when $\beta_j = 0$ for all j, explicit schemes have the advantage that they are very easy to solve, however for a given Δx , explicit schemes require a large number of points per wavelength in order to be accurate. Implicit schemes are more computationally demanding to solve allow us to use a larger Δx [2].

Dispersion Relation Preserving Schemes

Dispersion Relation Preserving (DRP) schemes minimize the error introduced by using the finite difference schemes for waves, by comparing the Fourier transform of the approximate derivative to the transform of the actual derivative. If they are similar then the dispersion relation of the wave, which determines many wave properties including the phase and group velocities, will be preserved. We can introduce an extra degrees of freedom by choosing to accept a larger truncation error, this then allows us to minimise the dispersion error with those degrees of freedom as parameters [1, 10, 14].

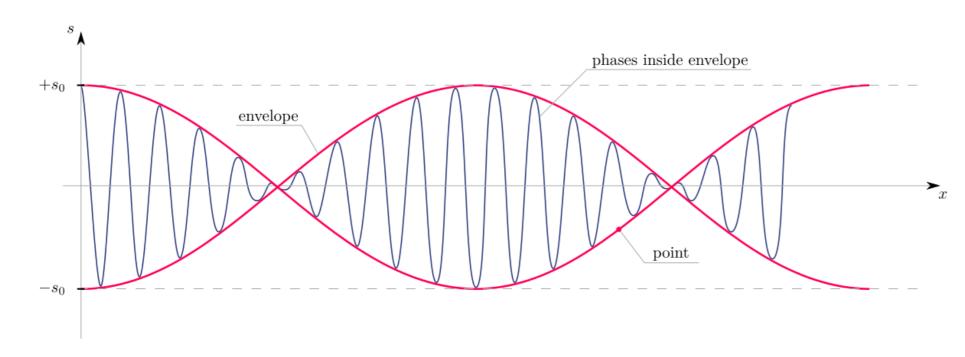


Figure 2: The interior wave propagates at the phase velocity, while the exterior wave propagates at the group velocity, both are determined by the dispersion relation $\omega = \omega(k)$.

For example, starting with a constant amplitude plane wave $u(x) = \Re(Ae^{i\alpha x})$, a general finite difference scheme gives us [3]:

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

This is our approximate wavenumber which we can then compare to the original wavenumber and minimise the error with any spare coefficients once the required accuracy conditions are satisfied.

Summation By Parts Schemes

At the boundaries of central finite difference schemes we run out of points to use in our approximations making it difficult to find higher order schemes which are stable close to the domain boundaries. In the continuous case, it is possible to show that upper and lower bounds on the energy exist by using integration by parts [12, 13]. We can write our general finite difference scheme (2) as:

$$Pu' \approx Qu$$
 (4)

Where u is the vector of u_i and u' is the vector of its first derivative. We pick P to be positive definite so that it defines an inner product, and Q, such that:

$$\langle \boldsymbol{u}, \boldsymbol{v} \rangle_P = \boldsymbol{u}^T P \boldsymbol{v}$$
 (5)

$$||\boldsymbol{u}||^2 = \boldsymbol{u}^T P \boldsymbol{u} \tag{6}$$

$$\int_{x}^{x_R} uvdx \approx \mathbf{u}^T P \mathbf{v} = \langle \mathbf{u}, \mathbf{v} \rangle_P \tag{7}$$

$$\implies Q + Q^T = E_n - E_0 = diag[0, ..., 0, 1] - diag[1, 0, ..., 0]$$
(8)

Where E_i are matrices who have 1 as the *ith* value of their diagonal and are zero elsewhere. When (5)-(7) hold, a property similar to integration by parts - known as summation by parts (SBP) - also holds. The integration by parts formula is:

$$\int_{\Omega} uvdx = uv|_{\Omega} - \int_{\Omega} v \frac{\partial u}{\partial x} dx \tag{9}$$

The discrete analog of this which (5)-(7) are necessary and sufficient for [12] is:

$$\langle \boldsymbol{u}, \boldsymbol{v} \rangle_P = \boldsymbol{u}^T (E_n - E_0) \boldsymbol{v} - \langle P^{-1} Q \boldsymbol{u}, \boldsymbol{v} \rangle_P$$
 (10)

This implies that an approximation scheme with conditions (5)-(7) will yield the same energy estimate as the analytical approach since we can use the same steps but use summation by parts instead of integration by parts, proving the approximation is time stable whenever the continuous case is time stable[7].

Results

The aim now is to construct a high order, implicit SBP scheme, preferably in such a way that we leave degrees of freedom available for DRP like optimization. Motivated by Carpenter, Gottlieb and Abarbanel's 1994 paper [5], in which they constructed an implicit fourth order scheme with third order accuracy at the boundaries, 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.

By exploiting symmetries we can write the SBP conditions as matrix equations. We first multiply (4) by H on each side and look to find H such that W = HP is symmetric and V = HQ satisfies (8). Considering just a 6×6 upper boundary block (which we denote using H, P and Q), we can write:

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

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

$$\text{Where } a, b, \text{ and } c \text{ are constants from the truncation accuracy conditions.}$$

From arranging these equations it became clear that, though counterintuitive, using a 7-point stencil would give simpler equations that a 5-point stencil. Using more matrix algebra we derived a set of non-linear equations which implicitly define a tri-diagonal, 6th order, 7 point, implicit SBP scheme including some free parameters which can be used for DRP-like optimization. The non-linear system is difficult to solve explicitly and so it is not yet possible to confirm whether the non linear system had solutions, nor test the performance of this new scheme against others.

Conclusions

- We analysed the theory and useful features of different types of finite difference schemes in an acoustical context.
- We determined the properties we wished to include in a new scheme.
- We outlined a systematic method for constructing a sixth order scheme and found that a 7 point stencil was optimal. This also left an additional degree of freedom to using in optimizing the scheme.
- The computational approach revealed that it was necessary for the scheme to be tridiagonal.
- We then reached an implicit form of the scheme with two free parameters. Unfortunately this form was non-linear and is yet to be solved.
- Future steps would be to solve the system and compare the schemes performance to other schemes using test functions, or to use similar methodology to derive higher order schemes.

References

- [1] Graham Ashcroft and Xin Zhang. Optimized prefactored compact schemes. Journal of Computational Physics, 190(2):459 477, 2003.
- [2] Gautum Biswas. Computational Fluid Dynamics. Alpha Science Intl Ltd, 2013.
- [3] E.J. Brambley. Optimized finite-difference (drp) schemes perform poorly for decaying or growing oscillations. Journal of Computational Physics, 324(Supplement C):258 - 274, 2016.
- [4] E.J. Brambley. Asymmetric finite differences for non-constant-amplitude waves. *International Congress On Sound and Vibration*, 2017.
- [5] Mark H. Carpenter, David Gottlieb, and Saul Abarbanel. Time-stable boundary conditions for finite-difference schemes solving hyperbolic systems: Methodology and application to high-order compact schemes. *Journal of Computational Physics*, 111(2):220 – 236, 1994.
- [6] D.M. Causon and C.G. Mingham. *Introductionary Finite Difference Methods for PDEs*. Ventus Publishing, 2010.
- [7] David C. Del Rey Fernandez, Jason E. Hicken, and David W. Zingg. Review of summation-by-parts operators with simultaneous approximation terms for the numerical solution of partial differential equations. *Computers & Fluids*, 95(Supplement C):171 – 196, 2014.
- [8] Stefan Johansson. High order finite difference operators with the summation by parts property based on drp schemes (unpublished). 2004.
- [9] H.O. Kreiss and G. Scherer. Finite element and finite difference methods for hyperbolic partial differential equations. In Carl de Boor, editor, Mathematical Aspects of Finite Elements in Partial Differential Equations, pages 195 – 212. Academic Press, 1974.
- [10] Sanjiva K. Lele. Compact finite difference schemes with spectral-like resolution. *Journal of Computational Physics*, 103(1):16 42, 1992.
- [11] Lloyd N. Trefethen. Group velocity in finite difference schemes. Society for Industrial and Applied Mathematics, 24, 04 1982.
- [12] Bo Strand. Summation by parts for finite difference approximations for d/dx. *Journal of Computational Physics*, 110(1):47 67, 1994.
- [13] Magnus Svard and Jan Nordstrom. Review of summation-by-parts schemes for initial-boundary-value problems. 268, 11 2013.
- [14] Christopher K.W. Tam and Jay C. Webb. Dispersion-relation-preserving finite difference schemes for computational acoustics. *Journal of Computational Physics*, 107(2):262 - 281, 1993.