CHAPTER 10

Finite difference methods revisited

1. Compact finite difference schemes

1.1. Construction by Taylor series expansions. Spectral methods have been shown to be very accurate methods in the computation of smooth solutions to PDE's. For a wide class of problems we are interested in high order approximation of the solution to a PDE but are not able to use a spectral method. Typical difficulties involve the appearance of complicated boundary conditions or some limited region of rapid variation in the solution which should be treated separately from the entire computational domain. Spectral methods are global methods and hence difficult to adapt locally. This difficulty has become overcome in recent years through the spectral element method but significant complications of method arise.

From spectral methods we can notice that the accurate evaluation of derivatives is based upon knowledge of the entire grid function not just a few adjoining values. This leads to the idea of extending a finite difference stencil to include more points. As we do this however the stencil becomes unwieldy encompessing perhaps a significant portion of the computational domain. We are interested in more accurate evaluations of the derivative but would like to keep the stencil compact. This has led to the application of Hermite polynomial interpolation ideas in which we seek the derivatives of a function $f(x)$ at the nodes of a uniform grid $\{x_j\}$ through formulas of the type

$$\frac{a}{2h}(f_{j+1}-f_{j-1})+\frac{b}{4h}(f_{j+2}-f_{j-2})+\frac{c}{6h}(f_{j+3}-f_{j-3}) = \beta f'_{j-2}+\alpha f'_{j-1}+f'_j+\alpha f'_{j+1}+\beta f'_{j+2} \tag{1.1}$$

Note that the computational stencil is widened and we have to solve a banded system to find the approximations of the derivative.

Taylor series expansions lead to relations among the coefficients introduced above

$$O(1): a+b+c = 2\beta+2\alpha+1 \tag{1.2}$$

$$O(h^2): \frac{a}{6}+\frac{2b}{3}+\frac{3c}{2} = 4\beta+\alpha \tag{1.3}$$

$$O(h^4): \frac{a}{120}+\frac{2b}{15}+\frac{27c}{40} = \frac{4\beta}{3}+\frac{\alpha}{12} \tag{1.4}$$

$$\cdots \tag{1.5}$$

The powers of h corresponding to each relation are indicated in (1.2-1.4). We obtain second order accuracy if we apply just the first relation (1.2), $O(h^4)$ accuracy if we apply the first 2 formulas and so on. Each relation adds another restriction to the values of available coefficients. There are 5 unknown coefficients in the set of equations above. For example, choosing just the first three relations leads to a two parameter family

$$a = \frac{1}{6}\alpha - \frac{10}{3}\beta + \frac{3}{2}, b = \frac{32}{15}\alpha + \frac{62}{15}\beta - \frac{3}{5}, c = \frac{6}{5}\beta - \frac{3}{10}\alpha + \frac{1}{10}\ . \tag{1.6}$$

In such a family of solutions we can impose additional constraints. Should we wish to solve a tridiagonal system for the derivatives we would impose $\beta = 0$ and obtain

$$a = \frac{1}{6}\alpha + \frac{3}{2},\ b = \frac{32}{15}\alpha - \frac{3}{5},\ c = -\frac{3}{10}\alpha + \frac{1}{10}\ . \tag{1.7}$$

Conversely, we might wish to obtain the smallest possible stencil for a given order of accuracy. This would lead to imposing $c = 0$ and the family

$$a = \frac{16}{9} - \frac{2}{3}\alpha,\ b = \frac{19}{6}\alpha - \frac{17}{18} \tag{1.8}$$

with $\beta = (3\alpha - 1)/12$. Thus we obtain a famil

Second derivatives are constructed throough a similar procedure

(1.9)
$$\frac{a}{h^2}(f_{j+1} - 2f_j + f_{j-1}) + \frac{b}{4h^2}(f_{j+2} - 2f_j + f_{j-2}) + \frac{c}{9h^2}(f_{j+3} - 2f_j + f_{j-3}) = \beta f''_{j-2} + \alpha f''_{j-1} + f''_j + \alpha f''_{j+1} + \beta f''_{j+2}$$

Taylor series expansions lead to the system

$$a + b + c = 2\alpha + 2\beta + 1 \tag{1.10}$$

$$\frac{a}{12} + \frac{b}{3} + \frac{3c}{4} = \alpha + 4\beta \tag{1.11}$$

$$\frac{a}{360} + \frac{2b}{45} + \frac{9c}{40} = \frac{\alpha}{12} + \frac{4\beta}{3} \tag{1.12}$$

with the two-parameter solution family

$$a = \frac{3}{2} - 3\beta - \frac{9}{4}\alpha, b = \frac{24}{5}\alpha - \frac{6}{5}\beta - \frac{3}{5}, c = \frac{31}{5}\beta - \frac{11}{20}\alpha + \frac{1}{10}\ . \tag{1.13}$$

1.2. Fourier analysis of compact finite difference schemes. The benefits of the procedure outlined above are shown by Fourier analysis of the ensuing finite difference formulas. Consider a periodic function $f(x + 2\pi) = f(x)$ and a uniform discretization $x_j = -\pi + jh$, $h = 2\pi/N$. The finite wavenumber, discrete Fourier series representing f on this grid is

$$f_j = \sum_{k=-N/2+1}^{N/2} \hat{f}_k \omega_N^{jk} \tag{1.14}$$

with $\omega_N = exp(2\pi i/N)$, the N^{th} root of unity. The full Fourier series representing the function is

$$f(x) = \sum_{k=-\infty}^{\infty} c_k e^{ikx} \tag{1.15}$$

and that representing its derivative is

$$f'(x) = \sum_{k=-\infty}^{\infty} ikc_k e^{ikx}\ . \tag{1.16}$$

Assume that N is large enough so all Fourier components of f and f' are captured on the finite representation and there is no aliasing error, i. e. $\hat{f}_k = c_k$ for $k = -N/2+1, \ldots, N/2$ and the derivative can be expressed as

$$f'_j = \sum_{k=-N/2+1}^{N/2} ik\hat{f}_k\omega_N^{jk} \tag{1.17}$$

We pose the problem of how well the Fourier representation of the derivative is approximated by various finite difference formulas. For instance the standard $O(h^2)$ centered formula leads to

$$f'_j \cong \frac{f_{j+1} - f_{j-1}}{2h} = \sum_{k=-N/2+1}^{N/2} \frac{i\sin kh}{h}\hat{f}_k\omega_N^{jk} \tag{1.18}$$

so the factor multiplying each Fourier coefficient is $i(\sin kh)/h$ instead of the exact factor ik. We can form a relative error

$$e(\kappa) = \left|\frac{\sin\kappa - \kappa}{\kappa}\right| = \left|\frac{A(\kappa) - \kappa}{\kappa}\right| \tag{1.19}$$

with $\kappa = kh$. A number of such expressions shall arise which will differ by $A(\kappa)$, the particular finite difference approximation of the correct Fourier differencing coefficient. For the family of schemes that result from imposing (1.1) we obtain

$$A(\kappa) = \frac{a\sin\kappa + (b/2)\sin 2\kappa + (c/3)\sin 3\kappa}{1 + 2\alpha\cos\kappa + 2\beta\cos 2\kappa}. \tag{1.20}$$

For a formula to reproduce as accurately as possible the Fourier representation of the derivative we would want $A(\kappa) = \kappa$. This may be used to impose additional constraints on the coefficients a, b, c, α, β. For instance we could construct the sum over the represented wavenumbers

$$S = \sum_{k=-N/2+1}^{N/2} \left[\frac{a\sin kh + (b/2)\sin 2kh + (c/3)\sin 3kh}{1 + 2\alpha\cos kh + 2\beta\cos 2kh} - kh\right]^2 \tag{1.21}$$

and minimize the this sum with respect to some of the coefficients to obtain additional restrictions.

A graphical representation of $A(\kappa)$ versus κ is most useful in interpretation of the quality of various finite difference approximations in Fourier space. Let us write down some particular $A(\kappa)$ expressions:

(1) Standard, $O(h^2)$ centered finite difference formula

$$A_1(\kappa) = \sin\kappa \tag{1.22}$$

(2) $O(h^4)$, compact stencil, tridiagonal system for f'

$$a = \alpha = -1,\ b = c = \beta = 0 \tag{1.23}$$

$$A_2(\kappa) = \frac{3\sin\kappa}{2+\cos\kappa} \tag{1.24}$$

(3) $O(h^6)$, tridiagonal system for f'

$$A_3(\kappa) = \frac{1}{3}(4 - \cos\kappa)\sin\kappa \tag{1.25}$$

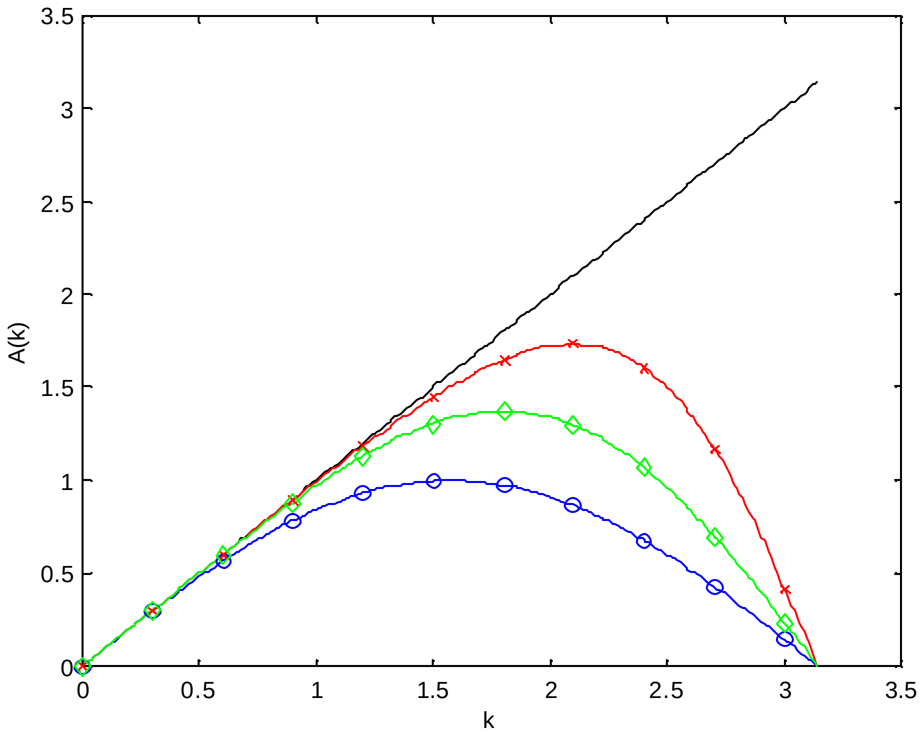

Figure 1. Accuracy in capture of wavemodes present in f^0 using various finite difference formulas. A_1 - circles, A_2 - x, A_3 - diamond.

This is shown in Fig. 1. The behavior of the exact Fourier coefficients of the derivative is shown by the $x = y$ line. We see that the standard $O(h^2)$ centered formula leads to large errors starting at $\kappa \gtrsim \pi/6$. The full range of wave numbers resolvable by the grid is from $\kappa = 0$ to $\kappa = \pi$. The largest wavenumber corresponds to the Nyquist criterion. We can interpret these findings as suggesting that when using the standard centered formula we are able to accurately resolve Fourier components if they are sampled with 6 times the number of points suggested by the Nyquist criterion, 12 points instead of 2. The formula corresponding to A_2 shows much better behavior, requiring only 6 sample points per wavelength, still more than the theoretical minimum given by the Nyquist criterion. The higher order compact finite difference formulas, optimized to reproduce the derivatives spectral behavior do reach the Nyquist limit, thus reproducing the desirable behavior of the spectral schemes.