Compact finite-difference schemes

Simulations of many of fluid mechanics related phenomena require high order of numerical accuracy and low numerical dissipation. Examples are turbulent flows where a wide range spatial scales need to resolved at the same time, and problems including acoustics. Examples of high accuracy methods are:

– Higher-order finite differences
– Spectral/Spectral Element methods
– Discontinuous Galerkin method
– High-Order Flux Reconstruction scheme

Beside the high numerical accuracy, the methods need also to be computationally efficient. Compact finite-difference method due to its narrow stencil is a good candidate for numerical applications requiring high accuracy. The method discussed here provide a family of discretization schemes which havs up to tenth-order of accuracy.

<u>*First derivative*</u>

Finite difference approximation to the derivative of a function is expressed as a linear combination of the given function values. In general form. this can be written as

$$\begin{aligned} f_i' \; + \; & \alpha(f_{i-1}' + f_{i+1}') + \beta(f_{i-2}' + f_{i+2}') = \\ & \frac{a}{2h}(f_{i+1} - f_{i-1}) + \frac{b}{4h}(f_{i+2} - f_{i-2}) + \frac{c}{6h}(f_{i+3} - f_{i-3}) \quad (*) \end{aligned}$$

The relation between coefficients a, b, c, α and β are derived matching the Taylor series coefficients of various order.

Expand f and f' around their values at x_i

$$f_{i\pm m} = f_i + \sum_{k=1}^{\infty} (\pm mh)^k \ \frac{1}{k!} \ f_i^{(k)}$$

$$f'_{i\pm m} = f'_i + \sum_{k=1}^{\infty} (\pm mh)^k \ \frac{1}{k!} \ f_i^{(k+1)}$$

where $f^{(k)} = \dfrac{d^k f}{dx^k}$

Insert expression above in $(*)$

$$\begin{aligned}
f'_i \ &+ \ \alpha \left(2f'_i + \sum_{k=1}^{\infty} \left[h^k + (-h)^k \right] \ \frac{1}{k!} \ f_i^{(k+1)} \right) \\
&+ \ \beta \left(2f'_i + \sum_{k=1}^{\infty} \left[(2h)^k + (-2h)^k \right] \ \frac{1}{k!} \ f_i^{(k+1)} \right) = \\
&\frac{a}{2h} \left(\sum_{k=1}^{\infty} \left[h^k - (-h)^k \right] \ \frac{1}{k!} \ f_i^{(k)} \right) \\
&+ \ \frac{b}{4h} \left(\sum_{k=1}^{\infty} \left[(2h)^k - (-2h)^k \right] \ \frac{1}{k!} \ f_i^{(k)} \right) \\
&+ \ \frac{c}{6h} \left(\sum_{k=1}^{\infty} \left[(3h)^k - (-3h)^k \right] \ \frac{1}{k!} \ f_i^{(k)} \right)
\end{aligned}$$

This can be simplyfied as

$$
\begin{aligned}
f_i' \;&+\; 2\alpha\left(f_i' + \sum_{k=1}^{\infty}\frac{h^{2k}}{(2k)!}\; f_i^{(2k+1)}\right)\\
&+\; 2\beta\left(f_i' + \sum_{k=1}^{\infty}\frac{(2h)^{2k}}{(2k)!}\; f_i^{(2k+1)}\right) = \\
&\quad\frac{a}{h}\left(\sum_{k=0}^{\infty}\frac{h^{2k+1}}{(2k+1)!}\; f_i^{(2k+1)}\right)\\
&+\; \frac{b}{2h}\left(\sum_{k=0}^{\infty}\frac{(2h)^{2k+1}}{(2k+1)!}\; f_i^{(2k+1)}\right)\\
&+\; \frac{c}{3h}\left(\sum_{k=0}^{\infty}\frac{(3h)^{2k+1}}{(2k+1)!}\; f_i^{(2k+1)}\right)
\end{aligned}
$$

Collect coefficients of different orders

$$
\begin{aligned}
h^0 &: \quad 1 + 2\alpha + 2\beta = a + b + c \qquad \Rightarrow \text{error} \sim \mathcal{O}(h^2)\\
h^2 &: \quad 2\frac{3!}{2!}(\alpha + 2^2\beta) = a + 2^2 b + 3^2 c \quad \Rightarrow \text{error} \sim \mathcal{O}(h^4)\\
h^4 &: \quad 2\frac{5!}{4!}(\alpha + 2^4\beta) = a + 2^4 b + 3^4 c \quad \Rightarrow \text{error} \sim \mathcal{O}(h^6)\\
h^6 &: \quad 2\frac{7!}{6!}(\alpha + 2^6\beta) = a + 2^6 b + 3^6 c \quad \Rightarrow \text{error} \sim \mathcal{O}(h^8)\\
h^8 &: \quad 2\frac{9!}{8!}(\alpha + 2^8\beta) = a + 2^8 b + 3^8 c \quad \Rightarrow \text{error} \sim \mathcal{O}(h^{10})
\end{aligned}
$$

These equations give different families of discretizations up to $\mathcal{O}(h^8)$

and a unique discretization for $\mathcal{O}(h^{10})$.

$c = b = \beta = 0 \quad \Rightarrow$ fourth order tridiagonal scheme (standard Padé scheme $\dfrac{f'_{i+1} + 4f'_i + f'_{i-1}}{6} = \dfrac{f_{i+1} - f_{i-1}}{2h}$)

$\alpha = \beta = 0 \quad \Rightarrow$ ordinary central-difference scheme ($c = 0$ penta diagonal 4th order $f'_i = \dfrac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12h}$)

($c = b = 0$ tridiagonal 2nd order $f'_i = \dfrac{f_{i+1} - f_{i-1}}{2h}$)

Fourier analysis of differencing errors

Assume periodic variables in $[0, L]$ and $h = L/N$

$$f(x) = \sum_{k=-N/2}^{N/2} \hat{f} e^{\left(\frac{2i\pi kx}{L}\right)} \quad \text{where } i = \sqrt{-1}$$

Introduce scaled wavenumber $\omega = \dfrac{2\pi kh}{L}$ and scaled coordinate $s = \dfrac{x}{h}$.

$$f(x) = \sum_k \hat{f}_k e^{i\omega s}, \quad \omega \in [0, \pi]$$

$$f'(x) = \sum_k \hat{f}'_k e^{i\omega s}, \quad \omega \in [0, \pi]$$

We have

$$f(x \pm mh) = \sum_k \hat{f} e^{\left(\frac{2i\pi kx}{L}\right)} e^{\left(\frac{\pm 2i\pi kmh}{L}\right)} = \sum_k \hat{f}_k e^{i\omega s} e^{\pm im\omega}$$

and

$$\frac{df}{dx} = \frac{ds}{dx}\frac{df}{ds} = \frac{1}{h}\sum_k \hat{f}'_k \; e^{i\omega s}$$

Insert in $(*)$

$$\begin{aligned} \frac{1}{h}\sum_k \hat{f}'_k \; e^{i\omega s} \;\; &+ \;\; \frac{\alpha}{h}\left[\sum_k \hat{f}'_k \; e^{i\omega s}(e^{i\omega} + e^{-i\omega})\right] \\ &+ \;\; \frac{\beta}{h}\left[\sum_k \hat{f}'_k \; e^{i\omega s}(e^{2i\omega} + e^{-2i\omega})\right] = \\ & \;\; \frac{a}{2h}\left[\sum_k \hat{f}_k \; e^{i\omega s}(e^{i\omega} - e^{-i\omega})\right] \\ &+ \;\; \frac{b}{4h}\left[\sum_k \hat{f}_k \; e^{i\omega s}(e^{2i\omega} - e^{-2i\omega})\right] \\ &+ \;\; \frac{c}{6h}\left[\sum_k \hat{f}_k \; e^{i\omega s}(e^{3i\omega} - e^{-3i\omega})\right] \end{aligned}$$

After simplifications

$$\hat{f}'_k\left[1 + 2\alpha\cos(\omega) + 2\beta\cos(2\omega)\right] = -i\hat{f}_k\left[a\sin(\omega) + \frac{b}{2}\sin(2\omega) + \frac{c}{3}\sin(3\omega)\right]$$

We know that the exact first derivative of the Fourier amplitudes are

$$(\hat{f}'_k)_{exact} = i\omega\hat{f} \Rightarrow \omega = \frac{(\hat{f}'_k)_{exact}}{i\hat{f}_k}$$

Define the modified wavenumber $\hat{\omega}$ as

$$\hat{\omega} = \frac{\hat{f}'_k}{i\hat{f}_k}$$

Here. we have

$$\hat{\omega} = \frac{a\sin(\omega) + \frac{b}{2}\sin(2\omega) + \frac{c}{3}\sin(3\omega)}{1 + 2\alpha\cos(\omega) + 2\beta\cos(2\omega)}$$

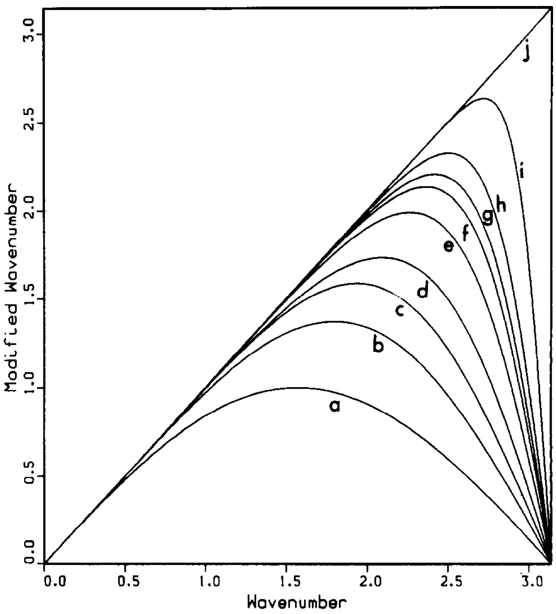

FIG. 1. Plot of modified wavenumber vs wavenumber for first derivative approximations: (a) second-order central differences; (b) fourth-order central differences; (c) sixth-order central differences; (d) standard Padé scheme ($\beta=0=c$, $\alpha=\frac{1}{4}$); (e) sixth-order tridiagonal scheme ($\beta=0=c$, $\alpha=\frac{1}{3}$); (f) eighth-order tridiagonal scheme ($\beta=0$); (g) eighth-order pentadiagonal scheme ($c=0$); (h) tenth-order pentadiagonal scheme; (i) spectral-like pentadiagonal scheme (3.1.6); (j) exact differentiation.

From S. K. Lele, *J. Computational Physics*, 103, 16–42 (1992)

The figure above shows that the compact scheme with same formal accuracy is found for narrower stencils compared to the traditional discretization scheme. It also shows that the compact schemes have a better spectral resolution, namely they are capable of resolving structures with smaller length scales for a given number of grid points. The spectral-like pentadiagonal scheme (i) is found by choosing the parameters such

$$\hat{\omega}(\omega_1) = \omega_1, \ \hat{\omega}(\omega_2) = \omega_2, \ \hat{\omega}(\omega_3) = \omega_3.$$

Results presented in figure above is found by choosing $\omega_1 = 2.2$, $\omega_2 = 2.3$ and $\omega_3 = 2.4$.