Compact finite-difference schemes

- What are they?

  Implicit, high-resolution finite-difference schemes. Also interpolation, filtering...

- What are they meant for?

  Improved resolution w.r.t. explicit finite-difference schemes, while maintaining a limited "stencil". Mainly used for DNS or LES of turbulent flows in simple geometries

- Fake claims:

  "CDSs are more suited than spectral methods to deal with complex geometries and arbitrary boundary conditions".

- Derivations from CDSs: compact finite-volume schemes.

Approximation of first derivative.

- Explicit second- and fourth-order central differences yield an approximation f_i' to $\frac{df}{dx}(x_i)$ using the function values at nodes near x_i, namely (f_{i-1}, f_{i+1}) for the second-order and $(f_{i-2}, f_{i-1}, f_{i+1}, f_{i+2})$ for the fourth-order approximations. In the spectral methods, the value of f_i' depends on all values of f at nodes. Compact difference schemes are a sort of compromise between these two extremes.

- Consider an approximation of the form:

1) $$\beta f_{i-2}' + \alpha f_{i-1}' + f_i' + \alpha f_{i+1}' + \beta f_{i+2}'$$
$$= c\,\frac{f_{i+3} - f_{i-3}}{6h} + b\,\frac{f_{i+2} - f_{i-2}}{4h} + a\,\frac{f_{i+1} - f_{i-1}}{2h}$$

The coefficients α, β, a, b, c are derived by matching the Taylor series coefficients of various orders. The first un-matched coefficient determines the formal truncation error of the approximation.

The constraints are:

$$a + b + c = 1 + 2\alpha + 2\beta \qquad (2^{nd} \text{ order})$$

$$a + 2^2 b + 3^2 c = 2\frac{3!}{2!}(\alpha + 2^2\beta) \qquad (4^{th} \text{ order})$$

$$a + 2^4 b + 3^4 c = 2\frac{5!}{4!}(\alpha + 2^4\beta) \qquad (6^{th} \text{ order})$$

$$a + 2^6 b + 3^6 c = 2\frac{7!}{6!}(\alpha + 2^6\beta) \qquad (8^{th} \text{ order})$$

$$a + 2^8 b + 3^8 c = 2\frac{9!}{8!}(\alpha + 2^8\beta) \qquad (10^{th} \text{ order})$$

Some of the coefficients may be left "free", therefore resulting in families of compact difference schemes of given order.

For instance, consider $\beta = 0$, $c = 0$ and let α free. A family of 4^{th}-order schemes is obtained:

$$\beta = 0, \; a = \frac{2}{3}(\alpha + 2), \; b = \frac{1}{4}(4\alpha - 1), \; c = 0$$

The widest stencil needed within this class of schemes spans three nodes on the left-hand side of 1) and five nodes on the right-hand side.

Special representatives of this family are:

$\alpha = 0 \Rightarrow$ fourth-order, explicit scheme

$\alpha = 1/4 \Rightarrow$ classical 4^{th}-order, Padè scheme

$\alpha = 1/3 \Rightarrow$ 6^{th}-order accurate scheme.

With $\beta = 0$ and $c \neq 0$, a two-parameter family of fourth-order schemes is obtained or, alternatively, a <u>one-parameter family of 6^{th}-order schemes:</u>

$$\beta = 0 \qquad a = \frac{1}{6}(\alpha + 9)$$

$$b = \frac{1}{15}(32\alpha - 9) \qquad c = \frac{1}{10}(-3\alpha + 1)$$

Choosing $\alpha = \frac{3}{8}$ yields the 8^{th}-order representative of the 6^{th}-order family. This is the tridiagonal scheme with the highest formal accuracy within (1).

Choosing $\beta \neq 0$, we end up with:

- a 3-parameter (α, β, c) 4^{th}-order family
- a 2-parameter (α, β) 6^{th}-order family
- a 1-parameter (α) 8^{th}-order family
- a single 10^{th}-order scheme.

The coefficients for the 10^{th}-order scheme are:

$$\alpha = \frac{1}{2} \qquad \beta = \frac{1}{20} \qquad a = \frac{17}{12} \qquad b = \frac{101}{150} \qquad c = \frac{1}{100}$$

Approximation of second derivative

(D2) $$\beta f''_{i-2} + \alpha f''_{i-1} + f''_{i} + \alpha f''_{i+1} + \beta f''_{i+2} =$$

$$= c\,\frac{f_{i+3} - 2f_i + f_{i-3}}{9h^2} + b\,\frac{f_{i+2} - 2f_i + f_{i-2}}{4h^2}$$

$$+\, a\,\frac{f_{i+1} - 2f_i + f_{i-1}}{h^2}$$

The constraints arising from Taylor expansion and truncation error reduction are:

$$a + 2^{2k} b + 3^{2k} c = \frac{(2k)!}{(2k-2)!}\left(\alpha + 2^{2k}\beta\right), \quad 2k\text{-th order}$$

$$k = 1, 2, 3, 4, 5$$

We consider only some special families and representatives of this broad class of schemes.

* 1-parameter family of 4^{th}-order schemes:

$$\beta = 0,\ c = 0,\ a = \frac{4}{3}(1-\alpha),\ b = \frac{1}{3}(-1+10\alpha)$$

$\alpha = \frac{1}{10}$ yields the classical Padé scheme ($b=0$).

* $\alpha = \frac{2}{11}$ yields a 6^{th}-order, tridiagonal scheme
($\beta = 0,\ a = \frac{12}{11},\ b = \frac{3}{11},\ c = 0$)

* 1-parameter 8-th order family:

$$\beta = \frac{38\alpha - 9}{214} \qquad a = \frac{696 - 1191\alpha}{428}$$

$$b = \frac{2454\alpha - 294}{535} \qquad c = \frac{1179\alpha - 344}{2140}$$

* 10^{th} order scheme:

$$\beta = \frac{43}{1798} \qquad \alpha = \frac{334}{899} \qquad a = \frac{1065}{1798}$$

$$b = \frac{1038}{899} \qquad c = \frac{79}{1798}$$

Fourier analysis of errors ("resolution")

For the purpose of Fourier analysis the dependent variables are assumed to be periodic over the domain $[0, L]$ of the independent variable, i.e., $f_1 = f_{N+1}$ and $h = L/N$. The dependent variables may be decomposed into their Fourier coefficients:

$$(1') \quad f(x) = \sum_{k=-N/2}^{N/2} \hat{f}_k \, e^{2\pi i \frac{kx}{L}}$$

Since $f(x)$ is a real-valued function, then

$$(2) \qquad \hat{f}_k = \hat{f}^{*}_{-k}, \quad 1 \le k \le N/2$$

and

$$\hat{f}_0 = \hat{f}^{*}_0$$

It is convenient to introduce a "scaled", or "modified" wavenumber w, defined as

$$w \equiv \frac{2\pi k h}{L} = \frac{2\pi k}{N}$$

w ranges from $-\pi$ to $+\pi$ but, due to the complex-conjugate correspondence (2), only the range $[0, \pi]$ is of interest.

Exact differentiation of (1') yields:

$$f'(x) = \sum_{k=-N/2}^{N/2} \hat{f}_k \, e^{\frac{2\pi i k x}{L}} \cdot \frac{2\pi i k}{L}$$

$$= \sum_{k=-N/2}^{N/2} i\omega \hat{f}_k \, e^{i\omega s}$$

where $s = x/h$. Thus, the Fourier coefficients of $f'(x)$ are $\hat{f}'_k = i\omega \hat{f}_k$.

The differencing error of the first derivative scheme may be assessed by comparing the Fourier coefficients of the derivative obtained from the differencing scheme $(\hat{f}'_k)_{fd}$ with the exact Fourier coefficients $\hat{f}'_k$.

The compact difference schemes for the first derivative presented above yield a modified wavenumber ω' so:

$$\left(\hat{f}'_k\right)_{fd} = i\omega' \hat{f}_k$$

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

Different schemes can be compared in terms of "resolving efficiency", i.e., the region of ω within which $\frac{|\omega' - \omega|}{\omega} \leq \varepsilon$, where ε is a pre-set tolerance.

An alternative view of dispersive error characteristics

Let's consider the transport equation:

$$\frac{\partial f}{\partial t} + c\frac{\partial f}{\partial x} = 0$$

$$x \in \mathbb{R}$$

$$t > 0$$

A general solution is $f(x-t)$, corresponding to a "waveform" shifting towards $+\infty$ with velocity c.

Considering a Fourier mode, $f = \sigma^{(t)} e^{i\omega s}$, we end up with:

$$0 = \dot{\sigma} + c\sigma i k \Rightarrow \sigma(t) = \sigma_0 e^{-ikct}$$

or

$$f(x,t) = \sigma_0 e^{ik(x-ct)}$$

$$= \sigma_0 e^{i\omega(s-ct/h)}$$

~~As for a finite-difference representation of the transport equation the solution at nodes turns out to be~~ can be expressed ~~in general form as:~~

$$\cancel{f_{f.d.}(x_j,t) = \sigma_0}$$

A finite-difference approximation of the transport equation yields:

$$\frac{\partial f}{\partial t} + c\frac{\delta f}{\delta x} = 0$$

$$\dot{\sigma} e^{ikx} + c\,ik' e^{ikx}\sigma = 0$$

$$\dot{\sigma}(t) = -ick'\sigma$$

$$\sigma(t) = \sigma_0 e^{-ick't}$$

$$\tilde{f}(x,t) = \sigma_0 e^{ik(x-ck'/k\,t)}$$

$$= \sigma_0 e^{i\omega(s-k'/k\,ct/h)}$$