Fundamentals about compact, finite-difference schemes and about linear interpolation shape functions

Chapter 1

Compact, finite-difference schemes

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:

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

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

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

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

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

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, Padé 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 one-parameter family of 6th-order schemes:

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

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

Choosing $\alpha = \frac{3}{8}$ yields the 8th-order representative of the 6th-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) 4th-order family
- a 2-parameter (α, β) 6th-order family
- a 1-parameter (α) 8th-order family
- a single 10th-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:

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

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

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

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

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

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

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

$\alpha=\frac{2}{11}$ yields a 6^{th}-order, tridiagonal scheme

$$\left(\beta=0,\ a=\frac{12}{11},\ b=\frac{3}{11},\ e=0\right)$$

* 1-parameter 8-th order family:

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

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

* 10-th order scheme:

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

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

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

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

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:

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

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

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' s:

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

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

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 tollerance.

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 modes turns out to be~~ : can be expressed ~~in general form as:~~

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

A finite-difference approximation of the transport equation yields:

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

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

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

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

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

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

The error introduced by the finite-difference approximation to the first derivative ~~term~~ is quantified by k'/k or by the "modified phase speed" $c' \equiv ck'/k$. Compact f.d. schemes or symmetric stencils result in a purely-real modif. phase speed, which in turn implies only "dispersion" but not dissipation. For completeness, let's consider the simplest upwind-based f.d. scheme, i.e. the 1st-order upwind scheme

$$\left.\frac{\delta f}{\delta x}\right|_j \simeq \frac{f_j - f_{j-1}}{h}$$

$$f = e^{ikx} \Rightarrow \left.\frac{\delta f}{\delta x}\right|_j = i k' e^{ikx}$$

$$k' = i \, \frac{\sin(kh/2)}{h/2} \, e^{-ikh/2}$$

$$\frac{k'}{k} = i \, \frac{\sin(w/2)}{w/2} \, e^{-iw/2}$$

~~The solution of the transport equation becomes:~~

~~semi-discrete~~

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

$$= \sigma_0 \, e^{ikx} \, e^{ictk\cdot(a+ib)}$$

$$= \sigma_0 \, e^{ikx} \, e^{i(ac)kt} \, e^{-bckt}$$

$$= \sigma_0 \, e^{ik(x-c't)} \, e^{-\tilde{\alpha} k^2 t}$$

$$\tilde{\alpha} = bc/k$$

$$\frac{k'}{k} = \frac{\sin \omega/2}{\omega/2} \cdot \left(\sin(\omega/2) + i \cos(\omega/2) \right)$$

$$= \frac{\sin^2(\omega/2)}{\omega/2} + i \, \frac{\sin(\omega)}{\omega}$$

$$\tilde{f}(x,t) = \sigma_0 \, e^{ik(x-c't)} \, e^{-\tilde{\alpha} k^2 t} \qquad (3)$$

$$\frac{c'}{c} = R(\omega)$$

$$k^2 \tilde{\alpha} = I c k$$

The real part of the modified wavenumber induces a dispersion error, while the imaginary part induces dissipation: the waveform is progressively damped as time passes by.

In order to provide a physical interpretation for I, let's consider the solution to the transport-diffusion equation

$$\frac{\partial f}{\partial t} + c\frac{\partial f}{\partial x} = \alpha \frac{\partial^2 f}{\partial x^2}$$

$x \in \mathbb{R}$

$t > 0$

$f(x,0) = \sigma_0 e^{ikx}$

$$\Rightarrow \quad \dot{\sigma} e^{ikx} + ick\sigma e^{ikx} = -\alpha k^2 \sigma e^{ikx}$$

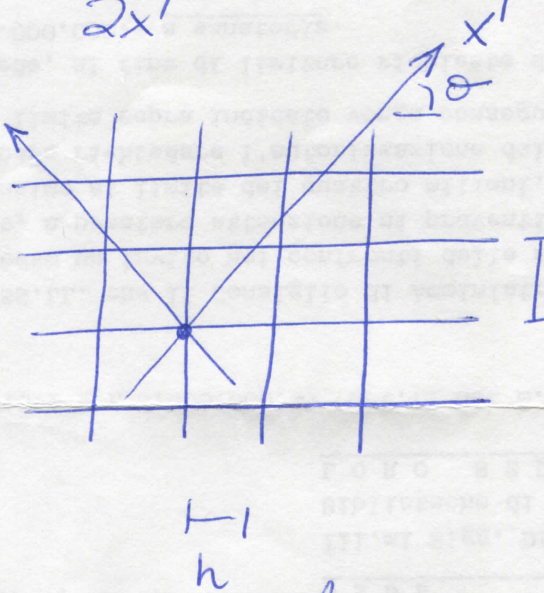
$$\Rightarrow \quad \dot{\sigma} + (ick - \alpha k^2)\sigma = 0$$

$$\Rightarrow \quad \sigma(t) = \sigma_0 e^{ik(x-ct)} e^{-\alpha k^2 t} \qquad (4)$$

Comparing (3) and (4) it turns out that the imaginary part of $\frac{k'}{k}$ corresponds to a "numerical diffusion" coefficient.

Anisotropy of a f.d. scheme deals with the representation of a Fourier mode, oriented along an off-grid direction. As for the transport equation, consider the following problem.

$$5)\quad \frac{\partial f}{\partial t} + c\,\frac{\partial f}{\partial x'} = 0$$



The general solution of (5) is:

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

When eq (5) is to be solved on a 2D, uniform Cartesian mesh ~~not oriented~~ not aligned with x', a coordinate mapping must be applied:

$$x' = x\cos\theta + y\sin\theta$$

$$y' = -x\sin\theta + y\cos\theta$$

The corresponding PDE reads:

$$\frac{\partial f}{\partial t} + c\left[\frac{\partial f}{\partial x}\cos\theta + \frac{\partial f}{\partial y}\sin\theta\right] = 0$$

with initial condition.

$$f(x,y,0) = \sigma_0 e^{iK(x\cos\theta + y\sin\theta)}$$

$$= \sigma_0 e^{i[(K\cos\theta)x + (K\sin\theta)y]}$$

Looking for a $f_\gamma^{d.}$ solution in the form

$$\tilde{f}(x,y,t) = \sigma(t)\, e^{i[(K\cos\theta)x + (K\sin\theta)y]}$$

yields

$$\mathring{\sigma} + \left[c\, i\, K'(K\cos\theta)\cos\theta + c\, i\, K'(K\sin\theta)\sin\theta\right]\sigma = 0$$

$\Rightarrow$ ~~$\tilde{f}(x,y,t) = \sigma_0 e^{i}$~~

or

$$\mathring{\sigma} + i c K'_{eff}\, \sigma = 0$$

$$\Rightarrow \quad \sigma(t) = \sigma_0 e^{-icK'_{eff}t}$$

$$\Rightarrow \tilde{\rho}(x,y,t) = \rho_0 e^{ik\left[x' - c_{f.d.} t\right]}$$

$$C_{f.d.} = c\,\frac{K'_{eff}}{K}$$

$$\frac{C_{f.d.}}{c} = \frac{K'(K\cos\theta)\cos\theta + K'(K\sin\theta)\sin\theta}{K}$$

$$= \frac{w'(w\cos\theta)\cos\theta + w'(w\sin\theta)\sin\theta}{w}$$

Considering for instance the second-order central finite difference:

$$w'(w) = \sin(w)$$

$$\frac{C_{f.d.}}{c} = \left[\sin(w\cos\theta)\cdot\cos\theta + \sin(w\sin\theta)\sin\theta\right]$$

$$\cdot\frac{1}{w} = \frac{\sin(w\cos\theta)\cos\theta}{w} + \frac{\sin(w\sin\theta)\sin\theta}{w}$$

It turns out that compact difference schemes have superior properties as regards anisotropy. For all considered schemes, the best resolution is obtained for $\theta = 45°$.

Resolving efficiency of second-order differencing scheme.

$$\frac{\delta^2 f}{\delta x^2} = -k_{eff}^2 \, e^{ikx}$$

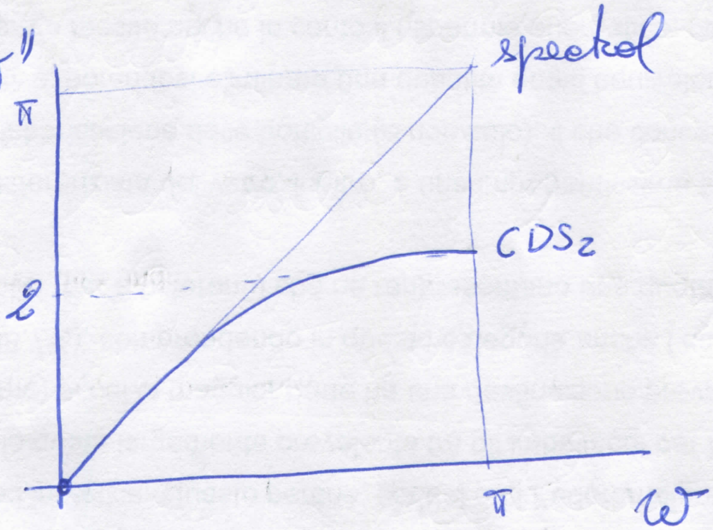
For instance for the CDS:

$$\left.\frac{\delta^2 e^{ikx}}{\delta x^2}\right|_j = \frac{e^{ikh} - 2 + e^{-ikh}}{h^2} \, e^{ikx_j}$$

$$= \frac{2\cos(kh) - 2}{h^2} \, e^{ikx_j}$$

$$K_{eff}^2 = \frac{2 - 2\cos(kh)}{h^2}$$

$$\left((kh)''\right)^2 \equiv \omega''^2 = 2\left(1 - \cos(kh)\right)$$



The modified wavenumber for compact difference schemes of type (D2) results in:

$$(\omega'')^2 = \frac{2a(1-\cos\omega) + (b/2)(1-\cos(2\omega)) + (2c/9)(1-\cos 3\omega)}{1 + 2\alpha\cos\omega + 2\beta\cos 2\omega}$$

NON-PERIODIC BOUNDARIES

Non-symmetric formulations for the first and second derivatives must be derived near boundary nodes.

As for the first derivative, consider for the boundary node

$i=1$:

$$f_1' + \alpha f_2' = \frac{1}{h}\left(a f_1 + b f_2 + c f_3 + d f_4\right)$$

$$\left.\begin{aligned} a &= -\frac{3+\alpha+2d}{2} \\ b &= 2+3d \\ c &= -\frac{1-\alpha+6d}{2} \end{aligned}\right\} 2^{nd}\text{-order accurate}$$

$$\left.\begin{aligned} a &= -\frac{11+2\alpha}{6} \\ b &= \frac{6-\alpha}{2} \\ c &= \frac{2\alpha-3}{2} \\ d &= \frac{2-\alpha}{6} \end{aligned}\right\} 3^{rd}\text{-order accurate}$$

$$\left.\begin{aligned} &\alpha = 3 \quad a = -17/6 \\ &b = 3/2 \quad c = 3/2 \\ &d = -1/6 \end{aligned}\right\} 4^{th}\text{-order accurate.}$$

It turns out that for even-order schemes the leading-order truncation error is of dispersive type, while it is dissipative for odd-order schemes.

The modified wavenumber ω' for boundary schemes is in general complex. As already seen for the upwind-difference scheme, the real part of ω' corresponds to dispersive error, the imaginary part to dissipation error. Some of the boundary schemes for f' proposed by Lele (1991) show anti-dissipative behavior: nevertheless, Lele (1991) reports, by numerical evidence that the complete differencing scheme (interior + boundary) leads to stable solutions.

As for the second derivative, ~~[illegible]~~ Lele (1991) proposes a 3rd-order boundary scheme:

$$f''_1 + 11 f''_2 = \frac{1}{h^2}\left(13 f_1 - 27 f_2 + 15 f_3 - f_4\right)$$

CONSERVATION PROPERTIES

Consider a conservation equation, e.g.:

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial x} F(f) = 0, \quad x \in [a,b]$$

or

$$\frac{\partial f}{\partial t} = \alpha \frac{\partial^2 F(f)}{\partial x^2}, \quad x \in [a,b]$$

Integrating over $[a,b]$:

$$\frac{d}{dt}\int_a^b f(x,t)\,dx = F\Big|_{(x=a,t)} - F\Big|_{(x=b,t)}$$

or

$$\frac{d}{dt}\int_a^b f(x,t)\,dx = \alpha \frac{\partial F}{\partial x}\Big|_{(x=b,t)} - \alpha \frac{\partial F}{\partial x}\Big|_{(x=a,t)}$$

The total f in the domain changes in time only due to the flux of f at the boundary. This is a global conservation statement.

Lele (1991) suggests to formulate the boundary schemes such that the global conservation property is retained by the difference approximations.

This approach also implies the appropriate quadrature weights for approximating the integral on l.h.s.

Let's consider the approximation for the first derivative, using different schemes for interior and boundary nodes. The schemes for the $\to$ $\boxed{\text{The coefficients for}}$ interior nodes may change from node to node.

$$\underline{\underline{A}}\,\underline{\hat{f}}' = \frac{1}{h}\,\underline{\underline{B}}\,\underline{\hat{f}}$$

$\underline{\underline{B}}, \underline{\underline{A}} \in \mathbb{R}^{N\times N}$, sparse; $\underline{\hat{f}}', \underline{\hat{f}} \in \mathbb{R}^{N-1}$

Lele (1991) states that "a sufficient condition for deriving a differencing scheme that satisfies the global conservation constraint is that the columns from 2 to $N-1$ of matrix $\underline{B}$ sum (row-wise) to zero".

Though Lele's derivation is rather confusing, I interpret this statement as follows:

$$\frac{\partial f}{\partial t} = -\frac{\partial F}{\partial x}$$

$$\downarrow$$

$$\underline{\dot{\hat{f}}} = -\underline{\underline{A}}^{-1}\underline{\underline{B}}\,\underline{F}$$

$$\Downarrow$$

$$\underline{\underline{A}}\,\underline{\dot{\hat{f}}} = -\underline{\underline{B}}\,\underline{F}$$

$$\Downarrow$$

$$\text{C1} \quad \boxed{\underline{w}^T\underline{\underline{A}}\,\underline{\dot{\hat{f}}} = -\underline{w}^T\underline{\underline{B}}\,\underline{F}}$$

$\underline{w}$: vector of weights

Equation C1 is (not explicitly!) used by Lele to enforce global conservation: ~~the~~ Lele determines the weights $\underline{w}$ and the coefficients of $\underline{\underline{B}}$ in such a way that $\underline{w}^T\underline{\underline{B}}\,\underline{F}$ depends only on F_1 and F_N. This is equivalent to require that

$$\underline{w}^T \underline{\underline{B}}_{:,2:N-1} = \underbrace{[0 - - - - - 0]}_{N-2 \text{ elements}}$$

and this is exactly the constraint used by Lele to derive schemes, ensuring global conservation.

global conservation constraints can be enforced for the second difference as well (see Lele § 4.3).

Eigenvalue analysis of the complete differencing scheme

This analysis is necessary to carry out a stability analysis of the overall differencing scheme.

$$
\begin{cases}
\dfrac{\partial f}{\partial t} + c\dfrac{\partial f}{\partial x} = 0 \\
x \in [0,1] \\
f(x=0,t) = 0 \qquad \text{(b.c.)}
\end{cases}
$$

$$\underline{\underline{A}}\,\underline{\hat{f}}' = \underline{\underline{B}}\,\underline{\hat{f}} \implies \frac{d\underline{\hat{f}}}{dt} = -\frac{c}{h}\underline{\underline{A}}^{-1}\underline{\underline{B}}\,\underline{\hat{f}}$$

$$\implies \underline{\underline{A}}\frac{d}{dt}\underline{\hat{f}} = -\frac{c}{h}\underline{\underline{B}}\,\underline{\hat{f}}$$

Consider a tentative solution:

$$\underline{\hat{f}} = e^{\sigma t}\,\underline{\tilde{f}}, \quad \sigma \in \mathbb{C}$$

$$\underline{\underline{A}}\,\sigma\,\underline{\tilde{f}} = -\frac{c}{h}\underline{\underline{B}}\,\underline{\tilde{f}}$$

$$\implies \underline{\underline{A}}^{-1}\underline{\underline{B}}\,\underline{\tilde{f}} = -\frac{\sigma h}{c}\underline{\tilde{f}}$$

In general, this eigenvalue problem must be solved numerically. In order the scheme to be stable, the real part of all "eigenvalues" σ must be negative.

<u>Remark</u>: we are carrying out a semi-discrete analysis. The effect of time-differentiation can be carried out analogously.

Stability analysis (using the von Neumann approach)

- For the transport equation:

$$\frac{\partial f}{\partial t} + c\,\frac{\partial f}{\partial x} = 0, \quad x \in \mathbb{R}$$

For a symmetric, compact difference scheme, $W' \equiv k_{eff}\, h \in \mathbb{R}^{+}$.

$$\frac{\partial \hat{f}}{\partial t} + \frac{i c w'}{h}\hat{f} = 0$$

Let $\sigma \equiv \dfrac{i c w'}{h}$. We are left with a set of ODEs. For a given, explicit time-stepping scheme, there exists a stability interval on the imaginary axis of the complex plane, for $\sigma \Delta t$.

Let $[-\sigma_i, +\sigma_i]$ be such an interval $(\sigma_i \in \mathbb{R}^{+} \cup \{0\})$.

The proposed scheme is stable as long as

$$\Delta t\, \frac{c}{h}\, \max(w') \leq \sigma_i$$

In other words, the CFL number has an upper bound for stability

$$CFL = \frac{c \Delta t}{h} \leq \frac{\sigma_i}{\max(w')}$$

Let's consider as an example a 3rd-order Runge-Kutta scheme, $\sigma_i = \sqrt{3}$, and a 4th-order Padé scheme for the first difference, providing

$$\max(w') = \sqrt{3} \quad \text{for } w = \frac{2\pi}{3}$$

The stability constraint reads thus:

$$CFL \leq \frac{\sqrt{3}}{\sqrt{3}} = 1$$

3rd-order Runge-Kutta:

$y' = f(t,y)$

$y_{n+1} = y_n + (K_1+4K_2+K_3)/6$

$K_1 = f(t_n,y_n)$

$K_2 = f(t_n+h/2, y_n+(h/2)K_1)$

$K_3 = f(t_{n+1}, y_n-hK_1+2hK_2)$

When f = f(t), this turns out to be Simpson's quadrature rule.

- Stability for the diffusion problem:

$$\frac{\partial f}{\partial t} = \nu \frac{\partial^2 f}{\partial x^2}$$

From the space discretization with a compact scheme for the second difference:

$$\frac{\partial \hat{f}}{\partial t} = - k_{eff}^2 \nu \hat{f}$$

$$= - \frac{(w^4)}{h^2} \nu \hat{f}$$

where $w^4 \equiv (k_{eff} h)^2$. In this case, the stability limit reads

$$\sigma_R^- \leq - \frac{w^4 \nu \Delta t}{h^2} \leq \sigma_R^+$$

where σ_R^- and σ_R^+ are the lower and upper bounds of the stability interval on the real axis. Notice that the exact solution of $\dot{f} = \sigma f$ diverges for $Re(\sigma) > 0$. Thus, we ~~are interested only~~ consider only the left inequality:

$$\frac{w^4 \nu \Delta t}{h^2} \leq |\sigma_R^-| \quad \forall w$$

which can be written as:

$$\boxed{\frac{\nu \Delta t}{h^2} \leq \frac{|\sigma_R^-|}{\max(\omega^4)}}$$

The dimensionless group $\frac{\nu \Delta t}{h^2}$ is a ratio of time-scales. Indeed, consider the damping by diffusion of a Fourier mode e^{ikx}:

$$e^{-\nu k^2 t} e^{ikx}$$

Thus, $1/(k^2 \nu) \sim L^2/\nu$ (L wavelength) corresponds to the time needed for the Fourier mode to be damped by a factor e^{-1}. In other words, L^2/ν is a time-scale for diffusion. The aforementioned stability constraint may be interpreted as a requirement that the time-step must be "smaller" than the time-scale of diffusion.

As a specific example, let's consider the Adams-Bashfort scheme for time-discretization and the 4^{th}-order Padé scheme for the second derivative,

$$\frac{1}{10} f''_{i-1} + f''_i + \frac{1}{10} f''_{i+1} = \frac{6}{5} \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2}$$

we find

$$\max(\omega''^{\,}) = \omega''(\omega = \pi) = 6$$

and $|\sigma_R| = 1$, yielding

$$\boxed{\frac{\nu \Delta t}{h^2} \le \frac{1}{6}}$$

As for the explicit, second-order difference scheme:

$$f''_i = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2}$$

$$\Rightarrow \max(\omega'') = \omega''(\omega = \pi) = 4$$

$$\boxed{\frac{\nu \Delta t}{h^2} \le \frac{1}{4}}$$

Two warnings:

1) The better the resolution features of a spatial discretization scheme are, the more stringent is the stability constraint for a given time-discretization scheme.

2) The stability limit on diffusion is in general more demanding than that on advection:

$$h \longrightarrow h' = h/2$$

$$\Rightarrow \Delta t \longrightarrow \Delta t' = \begin{cases} \Delta t/4 & \text{for diffusion} \\ \Delta t/2 & \text{for advection} \end{cases}$$

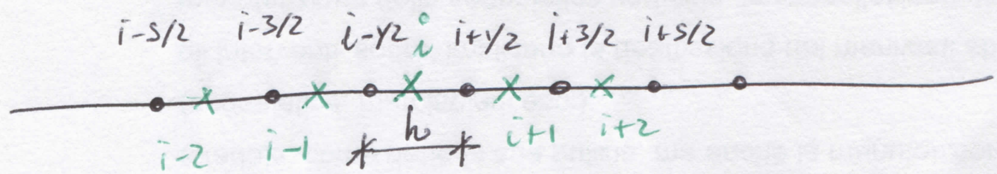
Interpolation and filtering

• Interpolation

$$\beta \hat{f}_{i-2} + \alpha \hat{f}_{i-1} + \hat{f}_i + \alpha \hat{f}_{i+1} + \beta \hat{f}_{i+2}$$

$$= \frac{c}{2}\left(f_{i+5/2} + f_{i-5/2}\right) + \frac{b}{2}\left(f_{i+3/2} + f_{i-3/2}\right)$$

$$+ \frac{a}{2}\left(f_{i+1/2} + f_{i-1/2}\right)$$



Taylor-series expansion yields the coefficients of different schemes.

The resolution of the scheme can be featured by a "transfer function" $T(\omega)$:

$$\hat{f}_i = T(\omega)\, e^{ikx_i}$$

For instance, for an explicit, second-order interpolation:

$$\hat{f}_i = \frac{f_{i+1/2} + f_{i-1/2}}{2}$$

$$\Rightarrow T(\omega)\, e^{ikx_i} = e^{ikx_i} \frac{e^{ikh/2} + e^{-ikh/2}}{2}$$

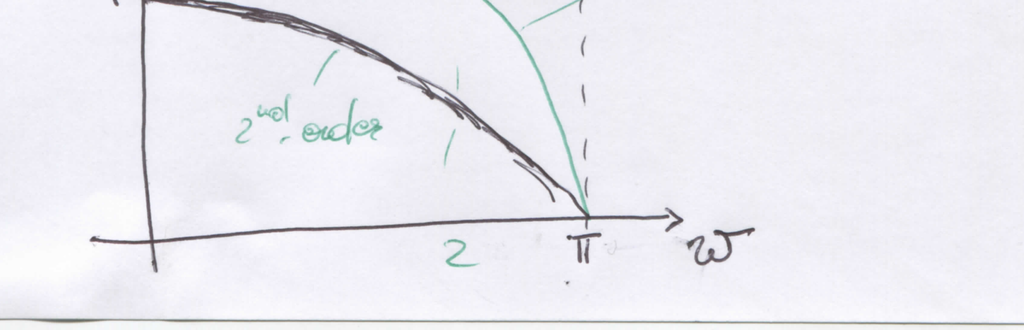
$$= e^{ikx_i} \cos(\omega/2)$$

$$\Rightarrow \boxed{T(\omega) = \cos(\omega/2)}$$

A 10^{th}-order compact scheme has coefficients:

$$\alpha = \frac{10}{21} \quad \beta = \frac{5}{126} \quad a = \frac{5}{3} \quad b = \frac{5}{14} \quad c = \frac{1}{126}$$

$$\boxed{T(\omega) = \frac{a\cos(\omega/2) + b\cos(3\omega/2) + c\cos(5\omega/2)}{1 + 2\alpha\cos\omega + 2\beta\cos(2\omega)}}$$



ω	$T(\omega)$	
	2^{nd} order	10^{th} order
0	1.000	1.000
$\pi/6$	0.966	1.000
$\pi/3$	0.866	1.000
$\pi/2$	0.707	1.000
$2/3\,\pi$	0.500	0.992
$5/6\,\pi$	0.259	0.868
π	0.000	0.000

1.1 Filtering

The idea is to filter out the high-wavenumber components of the solution vector $\boldsymbol{f}$, which are most likely related to numerical errors (as aliasing). Lele [1992] conceives filtering as a *in-place* interpolation:

$$\beta\,\widehat{f}_{i-2}+\alpha\,\widehat{f}_{i-1}+\widehat{f}_i+\alpha\,\widehat{f}_{i+1}+\beta\,\widehat{f}_{i+2} = a\,f_i+\frac{b}{2}\,(f_{i+1}+f_{i-1})+\frac{c}{2}\,(f_{i+2}+f_{i-2})+\frac{d}{2}\,(f_{i+3}+f_{i-3})$$

Taking the DFT of $\boldsymbol{f}$ and exploting orthonormality of the Fourier modes yields:

$$\widehat{f}_i = T(w)\,\mathrm{e}^{i\,w\,s_i}$$

where $w \equiv k\,h$ is the modified wavenumber and $s_i \equiv x_i/h$. The transfer function $T(w)$ reads:

$$T(w) = \frac{a + b\,\cos w + c\,\cos 2w + d\,\cos 3w}{1 + 2\,\alpha\,\cos w + 2\,\beta\cos 2w}$$

The formal accuracy of the filtering scheme is set by enforcing conditions on the derivatives at $w = 0$:

$$\left.\frac{\mathrm{d}^{(k)}T}{\mathrm{d}w^{(k)}}\right|_{w=0} = 0,\ k = 0,\,1,\,\ldots$$

Low-pass filtering conditions are reported by [Lele, 1992] in the form:

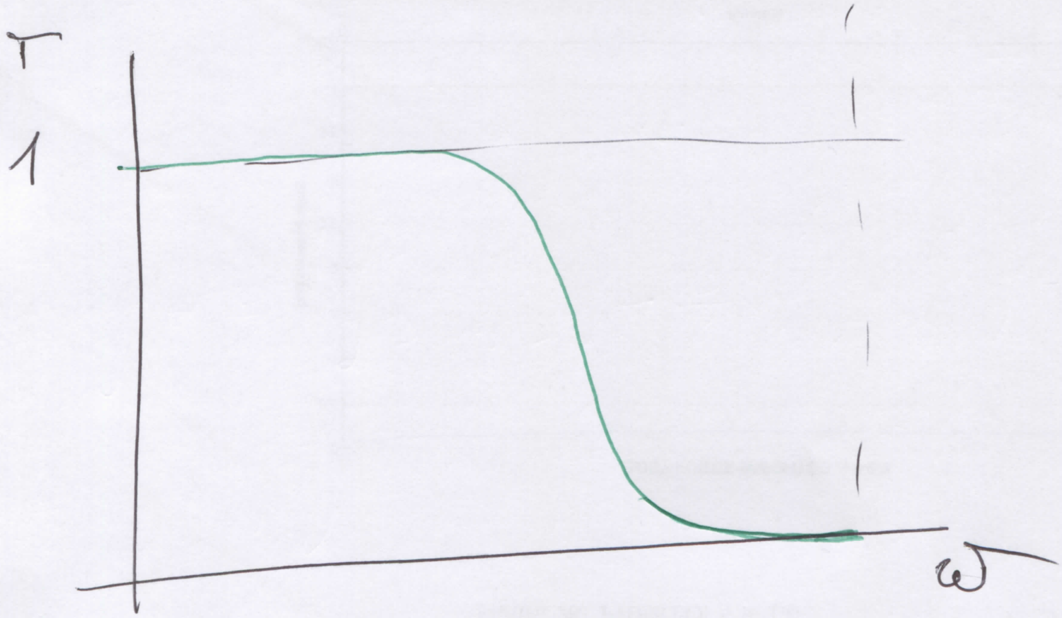
$$T(\pi) = 0; \quad T''(\pi) = 0; \quad T^{iv}(\pi) = 0$$

Each condition on the $2k$-th order derivative at $w = \pi$ automatically implies the vanishing of the derivative of order $2k + 1$ at $w = \pi$ (for symmetric schemes).

A 6^{th}-order filter satisfying all the filtering constraints is proposed by Dale (1991).

$\alpha = 0 \quad \beta = \frac{3}{10} \quad a = \frac{1}{2} \quad b = \frac{3}{4} \quad c = \frac{3}{10}$

$d = \frac{1}{20}$



ω	T(ω)
0	1.000
π/6	1.000
π/3	0.964
π/2	0.500
2/3 π	0.036
5/6 π	0.000
π	0.000

Boundary filters can be derived as well (see Lele, 1991, p 51)

Bibliography

J. Anderson. *Computational Fluid Dynamics*. Computational Fluid Dynamics: The Basics with Applications. McGraw-Hill Education, 1995. ISBN 9780070016859.

P.K. Kundu, I.M. Cohen, and D.R. Dowling. *Fluid Mechanics*. Elsevier Science, 2012. ISBN 9780123821003. URL https://books.google.it/books?id=iUo_4tsHQYUC.

K S Lele. Compact finite difference schems with spectral-like resolution. *J COMP PHYS*, 103:16–42, 1992.

M. Piller and E. Stalio. Finite-volume compact schemes on staggered grids. *J. Comp. Phys.*, 197(1):299 – 340, June 2004.

M. Piller and E. Stalio. Compact finite volume schemes on boundary-fitted grids. *J. Comp. Phys.*, 227(9):4736–4762, April 2008.

S.B. Pope. *Turbulent Flows*. Cambridge University Press, 2000. ISBN 9780521598866. URL https://books.google.it/books?id=HZsTw9SMx-0C.

J R Shewchuk. An introduction the conjugate gradient method without the agonizing pain. Technical report, School of Computer Science, Carnegie Mellon University, 1994.