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 an 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, Lele (1991) proposes a 3^{rd}-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
↳ $\boxed{\text{The coefficients for}}$
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; $\underline{\hat{f}}', \underline{\hat{f}} \in \mathbb{R}^{N\times 1}$

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 $\underline{\underline{B}}$ sum (row-wise) to zero".

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

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

$$\Downarrow$$

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

$$\Downarrow$$

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

$$\Downarrow$$

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

$\underline{w}$: 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

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

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.

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

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

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

Consider a tentative solution:

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

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

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

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 $\sigma \equiv \frac{i c w'}{h}$. 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 3^{rd}-order Runge-Kutta scheme, $\sigma_i = \sqrt{3}$, and a 4^{th}-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:

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

- 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 rewritten:

$$\boxed{\frac{\nu \Delta t}{h^2} \le \frac{|\omega_R^-|}{\max(\omega^u)}}$$

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 4th-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

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

As for the explicit, second-order difference scheme:

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

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

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

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:

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

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