

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 P' proposed by Lebe (1991) show ~~an~~ anti-dissipative behavior: nevertheless, Lebe (1991) reports ^{by} numerical evidence that the complete differencing scheme (interior + boundary) leads to stable solutions.

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

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

CONSERVATION PROPERTIES

Consider a conservation equation, e.g.:

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

or

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

Integrate over $[a, b]$:

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

or

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

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 ~~use~~ boundary schemes ~~in~~ formulate the

such ~~way~~ that the global conservation property is retained by the difference approximations.

~~This~~ This approach also implies the appropriate quadrature weights for ~~the~~ approximating the integral are $C_k \Delta x$.

Let's consider the approximation for the first derivative, using different schemes for interior and boundary nodes. ~~The~~ The scheme for the

interior nodes may change from node to node. \rightarrow The coefficients for

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

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

Lele (1991) states that "a sufficient condition for devising 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:

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



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



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



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

w: vector of weights

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

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

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

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

Eigensolver analysis of the complete differencing scheme

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

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

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

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

Consider a tentative solution:

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

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

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

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.

Remark: 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,
 $W' \equiv K_{\text{eff}} h \in \mathbb{R}^+$.

$$\frac{\partial \hat{f}}{\partial t} + \frac{icw'}{h} \hat{f} = 0$$

Let $\sigma \equiv \frac{icw'}{h}$. 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 ($\sigma_i \in \mathbb{R}^+ \setminus \{0\}$). 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

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

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

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

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 difference 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:

$$\begin{aligned} \frac{\partial \hat{f}}{\partial t} &= -K_{\text{eff}}^2 \nu \hat{f} \\ &= -\frac{(\omega^4)}{h^2} \nu \hat{f} \end{aligned}$$

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

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

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

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

which can be recast as:

$$\boxed{\frac{\nu \Delta t}{h^2} \leq \frac{|\mathbf{G}_R|}{\max(\omega^u)}}$$

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~~ 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~~ 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-Bashforth scheme for time-stepping and the 4th-order Runge-Kutta scheme for the second derivative,

$$\frac{1}{10} p_i^4 + p_i^4 + \frac{1}{10} p_{i+1}^4 = \frac{6}{5} \frac{p_{i+1} - 2p_i + p_{i-1}}{h^2}$$

we find

$$\max(\omega^4) = \omega^4(\omega = \pi) = 6$$

and $|\sigma_R| = 1$, yielding

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

As for the explicit, second-order difference scheme:

$$p_i^4 = \frac{p_{i+1} - 2p_i + p_{i-1}}{h^2}$$

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

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

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 for diffusion is in general more demanding than that for advection:

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