Appendix B

Numerical Analysis

B.1. Consistency

B.1.1. *Definitions*

The notion of consistency is applicable to the discretized version of a differential equation (see Chapters 6 and 7). It is defined in common language as follows.

A discretized equation is consistent with a differential equation if it becomes equivalent to it as the discretization space and time steps tend to zero. The "difference" between the original equation and the discretization is called the truncation error.

B.1.2. *Principle of a consistency analysis*

The following section explains how to carry out a consistency analysis. The example of the linear advection equation is used. The non-conservation form [1.48] of the linear advection is recalled here:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = 0$$

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Consider the first-order upwind discretization of equation [1.48] (see Chapter 6):

$$\left.\begin{aligned} C_i^{n+1} &= \mathrm{Cr}\, C_{i-1}^n + (1-\mathrm{Cr})C_i^n \\ \mathrm{Cr} &= \frac{u\Delta t}{\Delta x} \end{aligned}\right\} \qquad [B.1]$$

For the sake of clarity, let $C_i^n = C$. The consistency of [B.1] to [1.48] is analyzed using a second-order Taylor series expansion:

$$\left.\begin{aligned} C_{i-1}^n &= C - \Delta x \frac{\partial C}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 C}{\partial x^2} + \varepsilon_1(\Delta x^3) \\ C_i^{n+1} &= C + \Delta t \frac{\partial C}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 C}{\partial t^2} + \varepsilon_2(\Delta t^3) \end{aligned}\right\} \qquad [B.2]$$

Substituting equations [B.2] into equation [B.1] leads to:

$$\begin{aligned} &C + \Delta t \frac{\partial C}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 C}{\partial t^2} + \varepsilon_2(\Delta t^3) = (1-\mathrm{Cr})C \\ &\quad + \left[C - \Delta x \frac{\partial C}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 C}{\partial x^2} + \varepsilon_1(\Delta x^3) \right] \mathrm{Cr} \end{aligned} \qquad [B.3]$$

Substituting definition [B.1] of the Courant number into equation [B.3] yields the following equation:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = -\frac{\Delta t}{2}\frac{\partial^2 C}{\partial t^2} - \varepsilon_2(\Delta t^3) + u\frac{\Delta x}{2}\frac{\partial^2 C}{\partial x^2} + \frac{\varepsilon_1}{\Delta x}(\Delta x^3) \qquad [B.4]$$

The truncation error TE is defined as the difference between the discretized equation and the original equation. Comparing equations [1.48] and [B.4] leads to:

$$\mathrm{TE}(\Delta x, \Delta t) = -\frac{\Delta t}{2}\frac{\partial^2 C}{\partial t^2} - \varepsilon_2(\Delta t^3) + u\frac{\Delta x}{2}\frac{\partial^2 C}{\partial x^2} + \frac{\varepsilon_1}{\Delta x}(\Delta x^3) \qquad [B.5]$$

TE (Δx, Δt) tends to zero when both Δt and Δx tend to zero. Discretization [B.1] is consistent with the advection equation [1.48].

NOTE.– The truncation error contains powers of Δt and Δx. In contrast with a well-admitted (and incorrect) practice in engineering studies, decreasing only Δx or Δt is not sufficient for the discretization to be accurate. Both the time step and the cell size should be decreased in order to increase the accuracy of the discretization.

B.1.3. *Numerical diffusion, numerical dispersion*

Numerical diffusion and dispersion are purely numerical phenomena that arise from the discretization process. As seen in the previous section, the truncation error is made of an infinite sum of terms that contain powers of Δt and Δx multiplied by the derivatives of the solution with respect to time and/or space. TE (Δx, Δt) may be expressed in general form as:

$$\mathrm{TE}(\Delta x, \Delta t) = \sum_{p,q} \alpha_{p,q} \Delta t^{\beta_{p,q}} \Delta x^{\chi_{p,q}} \frac{\partial^{(p+q)} U}{\partial t^p \partial x^q} \qquad [B.6]$$

where the indices p and q vary from zero to infinity. Comparing equations [B.5] and [B.6] yields the following expressions for the coefficients $\alpha_{p,q}$ and the exponents $\beta_{p,q}$ and $\chi_{p,q}$:

$$\left.\begin{aligned} &\alpha_{1,0} = \alpha_{0,1} = \alpha_{1,1} = 0 \\ &\alpha_{2,0} = -\frac{\Delta t}{2} \\ &\alpha_{0,2} = \frac{\Delta x}{2} \\ &\beta_{2,0} = \beta_{0,2} = 1 \end{aligned}\right\} \qquad [B.7]$$

In general, $\beta_{p,q}$ and $\chi_{p,q}$ increase with p and q. The consequence is that the terms that contain higher-order derivatives decrease faster than those containing lower-order derivatives when Δt and Δx decrease. The relative importance of the lower-order terms in the truncation error increases when the cell size and the time step decrease.

Numerical diffusion appears when:

$$\left.\begin{aligned} &\alpha_{1,0} = \alpha_{0,1} = \alpha_{2,0} = \alpha_{1,1} = 0 \\ &\alpha_{0,2} \neq 0 \end{aligned}\right\} \qquad [B.8]$$

Then the lowest-order derivative in the truncation error is a second-order derivative with respect to x. Such a term is classically attached to diffusion, hence the term "numerical diffusion".

Numerical dispersion arises when the truncation error contains third-order derivatives with respect to space:

$$\left.\begin{array}{l} \alpha_{1,0} = \alpha_{0,1} = 0 \\ \alpha_{2,0} = \alpha_{1,1} = \alpha_{0,2} = 0 \\ \alpha_{3,0} = \alpha_{2,1} = \alpha_{1,2} = 0 \\ \alpha_{0,3} \neq 0 \end{array}\right\} \qquad [B.9]$$

Example: the truncation error [B.5] induces numerical diffusion. This can be shown by eliminating the second-order terms with respect to time. To do so, equation [B.4] is differentiated with respect to time and space:

$$\left.\begin{array}{l} \dfrac{\partial^2 C}{\partial t^2} + u\,\dfrac{\partial^2 C}{\partial x \partial t} = -\dfrac{\Delta t}{2}\dfrac{\partial^3 C}{\partial t^3} - \varepsilon_4(\Delta t^3) + u\,\dfrac{\Delta x}{2}\dfrac{\partial^3 C}{\partial x^2 \partial t} + \dfrac{\varepsilon_3}{\Delta x}(\Delta x^3) \\ \dfrac{\partial^2 C}{\partial x \partial t} + u\,\dfrac{\partial^2 C}{\partial x^2} = -\dfrac{\Delta t}{2}\dfrac{\partial^3 C}{\partial x \partial t^2} - \varepsilon_6(\Delta t^3) + u\,\dfrac{\Delta x}{2}\dfrac{\partial^3 C}{\partial x^3} + \dfrac{\varepsilon_5}{\Delta x}(\Delta x^3) \end{array}\right\} \qquad [B.10]$$

Eliminating the derivative $\partial^2 C / \partial x \partial t$ leads to a relationship between $\partial^2 C / \partial t^2$ and $\partial^2 C / \partial x^2$:

$$\begin{array}{l} \dfrac{\partial^2 C}{\partial t^2} = u^2\,\dfrac{\partial^2 C}{\partial x^2} + \left(u\,\dfrac{\partial^3 C}{\partial x \partial t^2} - \dfrac{\partial^3 C}{\partial t^3}\right)\dfrac{\Delta t}{2} + \left(\dfrac{\partial^3 C}{\partial x^2 \partial t} - u\,\dfrac{\partial^3 C}{\partial x^3}\right)\dfrac{u\Delta x}{2} \\ \qquad + \varepsilon_7(\Delta t^3) + \varepsilon_8(\Delta x^2) \end{array} \qquad [B.11]$$

Substituting equation [B.11] into equation [B.5] yields the following expression:

$$\mathrm{TE}(\Delta x, \Delta t) = \left(\frac{u\Delta x}{2} - \frac{\Delta t}{2}u^2\right)\frac{\partial^2 C}{\partial x^2} + [\varepsilon_9(\Delta t) + \varepsilon_{10}(\Delta x)]\Delta t \qquad [B.12]$$

where the polynomials ε_9 and ε_{10} contain third- and higher-order terms with respect to time and space. The first term on the right-hand side of the equal sign becomes predominant over the second term when Δt and Δx tend to zero, leading to the following equivalence:

$$\mathrm{TE}(\Delta x, \Delta t) \underset{\substack{\Delta x \to 0 \\ \Delta t \to 0}}{\approx} \left(\frac{u\Delta x}{2} - \frac{\Delta t}{2} u^2 \right) \frac{\partial^2 C}{\partial x^2} \qquad \text{[B.13]}$$

This is a diffusion term. The presence of this term in the truncation error indicates that the upwind scheme does not solve the linear advection [1.48] exactly, but an advection equation in the form:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} - D_{\mathrm{num}} \frac{\partial^2 C}{\partial x^2} \approx 0 \qquad \text{[B.14]}$$

where the numerical diffusion coefficient D_{num} is given as:

$$D_{\mathrm{num}} = \frac{u}{2}(\Delta x - u\Delta t) = (1 - \mathrm{Cr}) \frac{u\Delta x}{2} \qquad \text{[B.15]}$$

NOTE.– As indicated by the $\approx$ sign in equation [B.14], the truncation error contains higher-order terms in the polynomials ε_9 and ε_{10}. Consequently, the right-hand side of the equation is not strictly zero.

B.2. Stability

B.2.1. *Definition*

The notion of stability applies to the solution of a differential equation. The solution may be analytical or numerical.

A solution is said to be stable over the time-space domain $[x_1, x_2] \times [t_1, t_2]$ if it is bounded over the domain. In other words, there are two values $U_{\min}$ and $U_{\max}$ such that:

$$\exists (U_{\min}, U_{\max}), \quad U_{\min} \le U(x,t) \le U_{\max} \quad \forall \begin{cases} x \in [x_1, x_2] \\ t \in [t_1, t_2] \end{cases} \qquad \text{[B.16]}$$

For a numerical solution solved over a computational domain with M computational points for N computational time steps, the condition becomes:

$$\exists (U_{\min}, U_{\max}), \quad U_{\min} \le U_i^n \le U_{\max} \quad \forall \begin{cases} i = 1, \ldots, M \\ n = 1, \ldots, N \end{cases} \qquad \text{[B.17]}$$

Stability is usually referred to under the implicit assumption that there is no limit to the time interval over which the solution is to be computed. In other words, t_2 is assumed to be infinite.

B.2.2. *Principle of a stability analysis*

The simplest existing stability analysis technique is the harmonic stability analysis, also known as Von Neumann analysis. This method is applicable to linear equations with constant coefficients. The purpose is to investigate the stability of a solution that is to be computed from a known initial condition. Assume that the governing equation is an mth-order equation in the form:

$$\sum_{p=0}^{m} a_p \frac{\partial^p U}{\partial t^p} + b_p \frac{\partial^p U}{\partial x^p} = 0 \qquad \text{[B.18]}$$

where a_p and b_p are constant coefficients. The harmonic analysis consists of seeking solutions to equation [B.18] in the form of elementary harmonic solutions in the form:

$$U(x,t) = \sum_k u_k \exp(\omega_k t + \sigma_k x) = \sum_k U_k(x,t) \qquad \text{[B.19]}$$

where u_k is a constant and the coefficients σ_k and ω_k take the form:

$$\left.\begin{aligned} \sigma_k &= j\sigma_{k,i} \\ \omega_k &= \omega_{k,r} + j\omega_{k,i} \end{aligned}\right\} \qquad \text{[B.20]}$$

where j is the pure imaginary number, $j^2 = -1$. The numbers $\sigma_{k,r}$, $\omega_{k,r}$ and $\omega_{k,i}$ are real numbers. Therefore σ_k is a pure imaginary number, while ω_k is a complex number with real and imaginary parts. This is motivated by the following considerations. Substituting equation [B.20] into [B.19] leads to the following expression:

$$\begin{aligned} U_k(x,t) = {} & [\cos(\sigma_{k,i}x) + j\sin(\sigma_{k,i}x)]\times \\ & [\cos(\omega_{k,i}t) + j\sin(\omega_{k,i}t)]\exp(\omega_{k,r}t) \end{aligned} \qquad \text{[B.21]}$$

The elementary function U_k is a sinusoidal function of x (and is therefore periodic in space), the amplitude of which is a sinusoidal function of time multiplied by an exponential. The real part $\omega_{k,r}$ conditions the variation of the amplitude of the solution in time. If $\omega_{k,r}$ is negative, the amplitude of the solution decreases with time and the solution is stable. If $\omega_{k,r}$ is positive, the amplitude of the solution increases exponentially with time and the solution is unstable. The stability analysis thus amounts to studying the variations of $\omega_{k,r}$, more particularly its sign. Substituting equation [B.19] into equation [B.18] gives:

$$\sum_{p=0}^{m} a_p \frac{\partial^p \sum\limits_k U_k}{\partial t^p} + b_p \frac{\partial^p \sum\limits_k U_k}{\partial x^p} = 0 \tag{B.22}$$

Swapping the sums and using the linearity property of the differentiation operator gives:

$$\sum_k \left(\sum_{p=0}^{m} a_p \frac{\partial^p U_k}{\partial t^p} + b_p \frac{\partial^p U_k}{\partial x^p} \right) = 0 \tag{B.23}$$

Since the exponential functions U_k form an orthogonal set, no exponential can be expressed as a linear combination of other exponentials. Consequently, equation [B.23] leads to the necessary condition:

$$\sum_{p=0}^{m} a_p \frac{\partial^p U_k}{\partial t^p} + b_p \frac{\partial^p U_k}{\partial x^p} = 0 \qquad \forall k \tag{B.24}$$

In other words, equation [B.18] is applicable to each of the components U_k individually. Differentiating equation [B.19] with respect to time and space leads to:

$$\left.\begin{aligned} \frac{\partial^p U_k}{\partial t^p} &= \omega^p U_k \\ \frac{\partial^p U_k}{\partial x^p} &= \sigma^p U_k = (j\sigma_{k,i})^p U_k \end{aligned}\right\} \tag{B.25}$$

Substituting equation [B.25] into equation [B.24] leads to the following condition:

$$\sum_{p=0}^{m} a_p \omega^p + b_p \sigma^p = 0 \tag{B.26}$$

where the subscript k has been dropped for the sake of clarity. Solving equation [B.26] for a given value of σ yields R roots $\omega^{(r)}$ ($r = 1, \ldots, R$). The solution U_k then takes the form:

$$U_k(x,t) = \sum_{r=1}^{R} \beta^{(r)} \exp\left[\omega^{(r)} t + \sigma x\right] \qquad \text{[B.27]}$$

The solution is stable if and only if each of the exponentials in equation [B.27] are stable for all possible values of σ. In other words, the real part of each of the roots $\omega^{(r)}$ must be zero or negative.

B.2.3. *Harmonic analysis of analytical solutions*

B.2.3.1. *The linear advection equation*

The harmonic analysis of the advection equation in non-conservation form is carried out hereafter. The non-conservation form [1.48] is recalled:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = 0 \qquad \text{[B.28]}$$

This equation can be written in the form [B.18] by letting:

$$\left.\begin{aligned} m &= 1 \\ a_1 &= 1 \\ b_1 &= u \end{aligned}\right\} \qquad \text{[B.29]}$$

The solution is sought in the form [B.19]. Differentiating expression [B.19] with respect to time and space gives:

$$\left.\begin{aligned} \frac{\partial U_k}{\partial t} &= \omega U_k \\ \frac{\partial U_k}{\partial x} &= j\sigma_i U_k \end{aligned}\right\} \qquad \text{[B.30]}$$

Substituting equation [B.30] into equation [B.28] yields the following equation:

$$\omega = ju\sigma_i \qquad \text{[B.31]}$$

The solution takes the form:

$$U_k = \beta \exp[(ut - x) j\sigma_i] \qquad \text{[B.32]}$$

Two remarks can be made:

– The real part of the exponential is zero. The solution is stable, its amplitude is constant.

– The solution is invariant for dx = u dt. This is precisely the invariance property derived in Chapter 1. Moreover, the speed at which the solution travels does not depend on the wavelength.

These two remarks may be synthesized as follows: the solution is transported at the speed u. Neither its shape nor its amplitude are altered.

B.2.3.2. *The diffusion equation*

The diffusion equation can be written in the form:

$$\frac{\partial U}{\partial t} - D\frac{\partial^2 C}{\partial x^2} = 0 \qquad \text{[B.33]}$$

where the diffusion coefficient D is a real positive number. Equation [B.33] is rewritten in the form [B.18] with:

$$\left.\begin{aligned} m &= 2 \\ a_1 &= 1 \\ a_2 &= b_1 = 0 \\ b_2 &= -D \end{aligned}\right\} \qquad \text{[B.34]}$$

The solution is sought in the form [B.19]. Differentiating equation [B.19] with respect to time and space gives:

$$\left.\begin{aligned} \frac{\partial U_k}{\partial t} &= \omega U_k \\ \frac{\partial^2 U_k}{\partial x^2} &= -\sigma_i^2 U_k \end{aligned}\right\} \qquad \text{[B.35]}$$

Substituting equation [B.35] into equation [B.33] leads to:

$$\omega = -D\sigma_i^2 \qquad \text{[B.36]}$$

Hence the expression of the solution:

$$U_k = U \exp(-D\sigma_i^2 t + i\sigma_i x) \qquad \text{[B.37]}$$

Two remarks can be made:

– The analytical solution of the diffusion equation is stable. This is because D is assumed to be positive. A negative coefficient D would lead to a positive ω, thus yielding an increasing exponential and an unstable solution.

– Large values of σ_i correspond to short wavelengths. The shorter the wavelength, the steeper the exponential. In other words, the amplitude of short waves decreases faster with time than the amplitude of long waves. This explains why steep fronts and sharp gradients are smoothed out faster than long waves and mild profiles.

B.2.3.3. *The advection dispersion equation*

The advection dispersion equation is a third-order PDE in the form:

$$\frac{\partial U}{\partial t} + u\frac{\partial C}{\partial x} + \Omega\frac{\partial^3 C}{\partial x^3} = 0 \qquad \text{[B.38]}$$

where the coefficient Ω is called the dispersion coefficient. Equation [B.38] can be written in the form [B.18] by letting:

$$\left.\begin{aligned} m &= 3 \\ a_1 &= 1 \\ a_2 &= a_3 = b_2 = 0 \\ b_1 &= u \\ b_3 &= \Omega \end{aligned}\right\} \qquad \text{[B.39]}$$

The solution is sought in the form [B.19]. Differentiating equation [B.19] with respect to time and space leads to:

$$\left.\begin{aligned} \frac{\partial U_k}{\partial t} &= \omega U_k \\ \frac{\partial U_k}{\partial x} &= j\sigma_i U_k \\ \frac{\partial^3 U_k}{\partial x^3} &= -j\sigma_i^3 U_k \end{aligned}\right\} \qquad \text{[B.40]}$$

Substituting equations [B.40] into equation [B.38] leads to:

$$\omega = (u - \Omega\sigma_i^2)\sigma_i \qquad \text{[B.41]}$$

The solution U_k takes the form:

$$U_k = U \exp\left\{\left[(u - \Omega\sigma_i^2)t - x\right] \ j\sigma_i\right\} \qquad \text{[B.42]}$$

Note that:

– the real part of the exponential is zero. The solution is stable, its amplitude is constant in time;

– the solution [B.42] verifies the following invariance property:

$$\frac{\mathrm{d}U_k}{\mathrm{d}t} = 0 \qquad \text{for } \frac{\mathrm{d}x}{\mathrm{d}t} = u - \Omega\sigma_i^2 \qquad \text{[B.43]}$$

The elementary solution U_k is invariant along the characteristic of speed $u - \Omega\sigma_i^2$. In contrast with the advection equation, the travelling speed of the solution of the dispersion equation depends on the wavelength. Although the amplitude of the waves does not change, the various waves in the solution are shifted gradually with respect to each other, leading to oscillations in the solution. The oscillations are usually stronger in the neighborhood of steep fronts because shorter waves are characterized by larger values of σ_i, thus leading to stronger shifts.

B.2.4. *Harmonic analysis of numerical solutions*

This section deals with the harmonic analysis of numerical solutions. Consider the explicit upwind scheme presented in Chapter 6, defined as in equation [B.1], recalled hereafter:

$$\left.\begin{aligned} C_i^{n+1} &= \mathrm{Cr}\ C_{i-1}^n + (1-\mathrm{Cr})C_i^n \\ \mathrm{Cr} &= \frac{u\Delta t}{\Delta x} \end{aligned}\right\}$$

The stability of a harmonic component U_k of the numerical solution is analyzed. Noting that C_i^n is the value of the numerical solution at the abscissa $x_i = i\,\Delta x$ at the time $t^n = n\,\Delta t$, equation [B.19] leads to the following expression for $(U_k)_i^{n+1}$:

$$\begin{aligned}(U_k)_i^{n+1} &= u_k \exp(\omega t^{n+1} + \sigma x) \\ &= u_k \exp[\omega(t^n + \Delta t) + \sigma x] \\ &= (U_k)_i^n \exp(\omega \Delta t)\end{aligned} \qquad [B.44]$$

while the following expression is obtained for $(U_k)_{i-1}^n$:

$$(U_k)_{i-1}^n = (U_k)_i^n \exp(-\sigma \Delta x) \qquad [B.45]$$

with $s = j\ \sigma_i$. Substituting equations [B.44–45] into the numerical scheme [B.1], we obtain:

$$\exp(\omega \Delta t) = \mathrm{Cr} \exp(-\sigma \Delta x) + 1 - \mathrm{Cr} \qquad [B.46]$$

The quantity $\exp(\omega\Delta t)$ is the factor by which the solution is multiplied from one time step to the next. It is referred to as the numerical amplification factor A_N:

$$A_N = \exp(\omega \Delta t) = \frac{(U_k)_i^{n+1}}{(U_k)_i^n} \qquad [B.47]$$

The solution is stable if the modulus of the amplification factor is equal to or smaller than unity. If this is the case, the modulus of the solution decreases from one time step to the next and the solution is indeed stable. Conversely, if the modulus of the amplification factor is larger than unity the numerical solution is unstable. The stability analysis amounts to studying the variations in the modulus of A_N with σ. This is done using a graphical representation in the complex plane (Figure B.1).

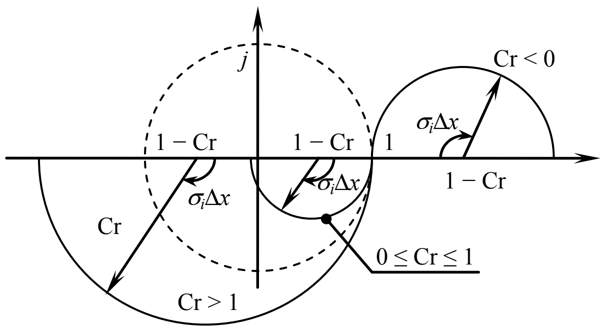

Figure B.1. *Definition sketch for the numerical amplification factor in the complex plane*

The expression for A_N is rewritten as:

$$A_N = 1 + [\exp(-\sigma\Delta x) - 1]\ \mathrm{Cr} \qquad [B.48]$$

The wave number M is introduced. M is the number of cells of width Δx needed to cover a period of the signal U_k:

$$M = \frac{2\pi}{\sigma_i \Delta x} \qquad [B.49]$$

The minimum possible value for M being 2 (at least two cells are needed to describe a sine wave), the quantity σ_i lies between 0 and π. A_N is represented graphically in the complex plane as the circle of radius |Cr] that is tangent to the unit circle at the point $z = 1$ (Figure B.1). The center of the circle is located at $z = 1 - \mathrm{Cr}$. Quite obviously, A_N is located outside the unit circle for $\mathrm{Cr} < 0$ and $\mathrm{Cr} > 1$. The solution is unstable. A_N is located inside the unit circle when Cr is between 0 and 1. In this case the numerical solution is stable.

B.2.5. *Amplitude and phase portraits*

Amplitude and phase portraits are graphical representations of the performance of numerical schemes. The amplitude and phase portrait display the modulus of the amplification factor and the numerical wave speed as functions of the wave number M respectively. The numerical wave speed is derived by noting that the solution component U_k is constant if:

$$\omega_{k,i}\mathrm{d}t + \sigma_{k,i}\mathrm{d}x = 0 \qquad [B.50]$$

In other words, U_k is an invariant along the characteristic line:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -\frac{\omega_{k,i}}{\sigma_{k,i}} = -\frac{\arg(A_N)}{\Delta t \sigma_{k,i}} = -\frac{M\Delta x \arg(A_N)}{2\pi\Delta t} \qquad [B.51]$$

The speed $\mathrm{d}x/\mathrm{d}t$ is usually referred to as the phase velocity (as opposed to the group velocity, see [VIC 82]). The ratio C_N of the numerical wave speed to the analytical wave speed is given by:

$$C_N = -\frac{M\Delta x \arg(A_N)}{2\pi u\Delta t} = -\frac{M \arg(A_N)}{2\pi \mathrm{Cr}} \qquad [B.52]$$

The amplification factor and the ratio of the wave speeds for the numerical solution of the advection equation must tend to one when the wave number tends to infinity. This is an indication that the numerical solution tends to behave as the analytical one when an infinity of points (hence and very small time step and cell width) are used to compute the numerical solution.

The amplitude portrait of the explicit upwind scheme [B.1] is obtained from equation [B.48] (see Figure B.2).

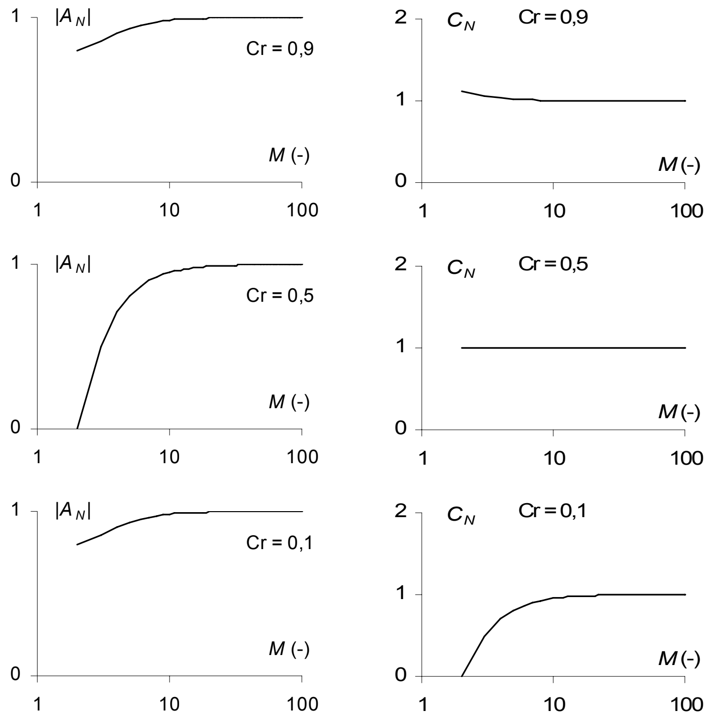

Figure B.2. *Amplitude and phase portrait for the explicit upwind scheme*

$$\begin{aligned} \left|A_N\right| &= \left|1 + [\cos(\sigma\Delta x) - 1 - j\sin(\sigma\Delta x)]\ \mathrm{Cr}\right| \\ &= \left\{[1 - \mathrm{Cr} + \mathrm{Cr}\cos(\sigma\Delta x)]^2 + [\mathrm{Cr}\sin(\sigma\Delta x)]^2\right\}^{1/2} \\ &= \left\{[1 - \mathrm{Cr} + \mathrm{Cr}\cos(2\pi / M)]^2 + [\mathrm{Cr}\sin(2\pi / M)]^2\right\}^{1/2} \end{aligned} \qquad \text{[B.53]}$$

The phase portrait is obtained from equations [B.48] and [B.52] (see Figure B.2):

$$C_N = -\frac{M \arg(A_N)}{2\pi u} = \frac{M \arccos(\mathrm{Re}\, A_N / |A_N|)}{2\pi u} \tag{B.54}$$

Note that:

– short waves are characterized by small wave numbers. The amplification factor being an increasing function of M, short waves are damped more quickly than long waves. After a certain amount of time, the shorter waves are eliminated from the numerical solution, only the longer waves remain. The most unfavorable configuration is encountered for $\mathrm{Cr} = 1/2$. In this case $A_N = 0$ for $M = 2$ and the waves $M = 2$ are eliminated from the numerical solution after the first time step. A first-order expansion in $1/M$ indicates in contrast that the amplification factor tends to one as M tends to infinity, which illustrates the convergence of the numerical solution toward the analytical solution;

– the numerical wave speed is larger than the analytical wave speed for Courant numbers larger than 1/2. It is smaller than the analytical wave speed for Courant numbers smaller than 1/2. C_N tends to unity as M tends to infinity, which is another indication that the numerical solution tends to the analytical one.

B.2.6. *Extension to systems of equations*

Harmonic analysis can be extended to systems of equations. When systems of equations are to be solved the solution is a vector variable and the amplification factor becomes a matrix. The eigenvalues of the matrix are complex in the general case. The solution is stable when the absolute value of each of the eigenvalues of the amplification factor is larger than one.

The stability analysis is carried out for the water hammer equations without source term. The non-conservation form [2.5] of the water hammer equations is recalled hereafter:

$$\frac{\partial \mathrm{U}}{\partial t} + \mathrm{A}\frac{\partial \mathrm{U}}{\partial x} = 0$$

where A and U are defined as in equations [2.68–69]:

$$\mathrm{A} = \begin{bmatrix} 0 & 1 \\ c^2 & 0 \end{bmatrix}, \qquad \mathrm{U} = \begin{bmatrix} \rho A \\ \rho Q \end{bmatrix}$$

The solution $U(x, t)$ is sought as the sum of elementary components U_k in the form:

$$U_k(x,t) = u_k \exp(\omega_k t + \sigma_k x) \qquad [B.55]$$

where u_k is a constant vector and the coefficients ω_k, σ_k are given as in equation [B.20]:

$$\left.\begin{aligned}\sigma_k &= j\sigma_{k,i}\\ \omega_k &= \omega_{k,r} + j\omega_{k,i}\end{aligned}\right\}$$

Differentiating equation [B.55] with respect to time and space gives:

$$\left.\begin{aligned}\frac{\partial U_k}{\partial t} &= \omega_k U_k\\ \frac{\partial U_k}{\partial x} &= j\sigma_{k,i} U_k\end{aligned}\right\} \qquad [B.56]$$

Substituting equations [B.56] into equation [2.5] leads to:

$$\omega_k \begin{bmatrix}\rho A\\ \rho Q\end{bmatrix} + \begin{bmatrix}0 & 1\\ c^2 & 0\end{bmatrix}\sigma_k \begin{bmatrix}\rho A\\ \rho Q\end{bmatrix} = 0 \qquad [B.57]$$

Equation [B.57] is rewritten as:

$$\begin{bmatrix}\omega_k & \sigma_k\\ c^2\sigma_k & \omega_k\end{bmatrix}\begin{bmatrix}\rho A\\ \rho Q\end{bmatrix} = 0 \qquad [B.58]$$

Equation [B.58] must hold for all possible values of U. This is true only if:

$$\begin{vmatrix}\omega_k & \sigma_k\\ c^2\sigma_k & \omega_k\end{vmatrix} = 0 \qquad [B.59]$$

that is:

$$\omega_k = \pm c\sigma_k \qquad [B.60]$$

The solution U_k is the sum of two exponential functions:

$$U_k(x,t) = u_k^{(1)} \exp[(x - ct)i\sigma_{k,i}] + u_k^{(2)} \exp[(x + ct)i\sigma_{k,i}] \qquad [B.61]$$

where $u_k^{(1)}$ and $u_k^{(2)}$ are constant vectors. Equation [B.61] allows the basic properties of the solution of the water hammer to be retrieved:

– The solution is the sum of two signals propagating at the speeds – *c* and + *c*.

– The arguments of the exponentials are pure imaginary numbers. Therefore the amplitude of the signals is constant. The solution is stable.

– The speed at which each of the signals propagates is independent of the wavelength of the elementary solution. The signals propagate without deformation in the pipe.

B.3. Convergence

B.3.1. *Definition*

The numerical solution of a differential equation is said to be convergent if it tends to the analytical solution as both the computational time step and the cell width tend to zero.

Engineers and modelers implicitly assume that convergence is true when they use software packages to solve the partial differential equations of engineering. The purpose indeed is that the numerical solution be as close to the exact solution as deemed appropriate given the objectives of the engineering project. This is achieved by decreasing the computational time step and the cell width until the numerical solution is considered accurate enough.

B.3.2. *Lax's theorem*

Convergence proofs are difficult to establish. They use notions in functional analysis that go beyond the usual mathematical apparatus accessible to engineers. Lax's theorem for linear equations with constant coefficients allows convergence to be related to consistency and stability. The theorem may be formulated as follows.

Consistency and stability are sufficient and necessary conditions to convergence.

In other words, if the governing equations are discretized in a consistent way and if the numerical solution is stable, then the numerical solution converges to the exact solution.