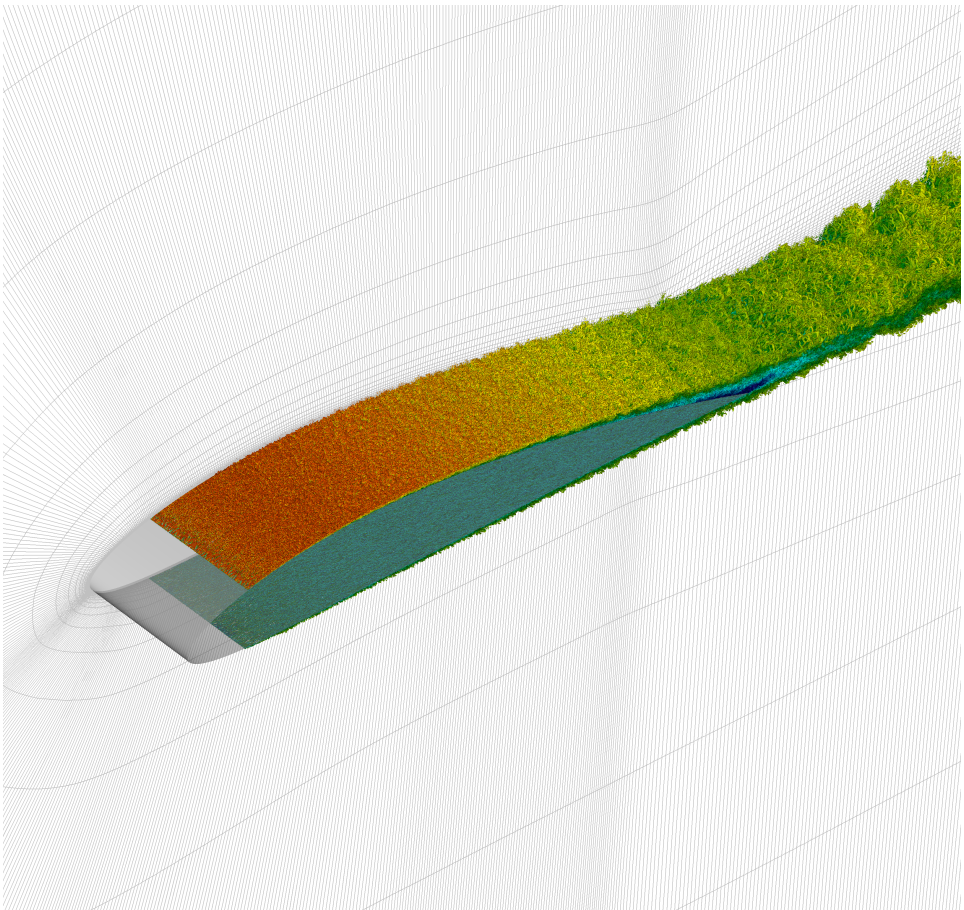
Lecture Notes
SG2212 / SG3114
Computational Fluid Dynamics
Part I



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Foreword

This document summarises the lectures on basic numerics, compressible flows and hyperbolic systems given within the course SG2212/SG3114 "Computational Fluid Dynamics" at KTH Royal Institute of Technology, Stockholm, Sweden. It is based on previous lectures notes used in the course, but was first typed up in LaTeX in 2019 and will be constantly updated. If there are any errors, unclear statements or typos, please contact Philipp Schlatter (`pschlatt@mech.kth.se`).

This document was put together by Alvaro Tanarro, Marco Atzori and Philipp Schlatter.

1 Type classification

1.1 Typical CFD problem

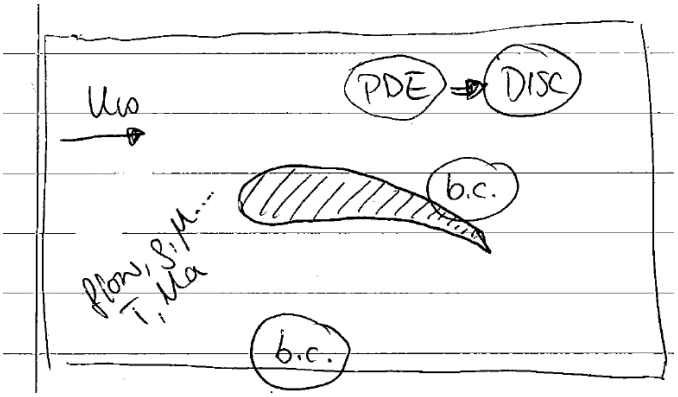


Figure 1.1: Sequence to solve a typical CFD problem.

The sequence to solve a typical CFD problem (or any engineering problem) is shown in Fig. 1.1:

1. physical problem: geometry, *etc.* based on experiments, experience, requirements.
2. physical model: approximation, which equation to use, ρ, μ, Ma, ...
3. mathematical model: PDE, BC, *etc.*
4. discretisation: method to use, FD
5. solution scheme, programming
6. calculation on a computer (see for instance `www.top500.org`)
7. validation, error analysis, postprocessing.

In particular the last step, *i.e.* the careful analysis of the results, might indicate changes in the setup, the equations, resolution *etc.* Already discussed: Steps 1-2 (Fluid Courses)

Now: steps 3-4 { model equations; classification, (math & physical); discretisation with FD

Later: Steps 5-7 (homeworks, project)

1.2 Model equations and classifications

- Solutions to different kinds of problems or equations behave differently.
- Choice of the numerical method depends on the equation to solve.
- Number, type and location of boundary conditions (b.c.) and initial conditions (i.c.) dependent on problem.

Definition 1.1 ***Well-posedness*:** (Hadamard 1902, natural problems) A system of PDEs and b.c./i.c. is a well-posed problem if:

1. a solution exists,
2. the solution is unique,
3. the solution depends continuously on the boundary and initial conditions.

Point 3 depends on the type of PDE.
A solution to a problem that is not well-posed (ill-posed) does not make sense and should not be attempted at all. □

Example 1.1 ***Backward heat equation*:** Consider the following PDE which is the normal heat equation with inverted sign for the diffusive term,

$$\frac{\partial u}{\partial t} = -\nu \frac{\partial^2 u}{\partial x^2} \qquad \nu > 0 \; . \tag{1.1}$$

The solution of this equation leads to unbounded amplification of errors (see also Section 4.3), and is thus not well posed (violates point 3). □

1.3 Classification of PDEs

System of linear, first order PDEs of two variables x, y with n unknowns $u_1, ..., u_n$,

$$\mathbf{A}\frac{\partial \underline{u}}{\partial x} + \mathbf{B}\frac{\partial \underline{u}}{\partial y} = \underline{c} \; . \tag{1.2}$$

Assume a curve $f(x, y) = 0$ in the two-dimensional (x, y) plane with specific parametrisation s, as shown in Fig. 1.2:

$$x = x(s) \, , \quad y = y(s) \tag{1.3}$$

Total derivative:

$$\frac{\mathrm{d}\underline{u}}{\mathrm{d}s} = \frac{\partial \underline{u}}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}s} + \frac{\partial \underline{u}}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}s} \tag{1.4}$$

Choose $s \equiv x$:

$$\frac{\mathrm{d}\underline{u}}{\mathrm{d}x}\Big|_f = \frac{\partial \underline{u}}{\partial x} + \frac{\mathrm{d}y}{\mathrm{d}x}\Big|_f \frac{\partial \underline{u}}{\partial y} \tag{1.5}$$

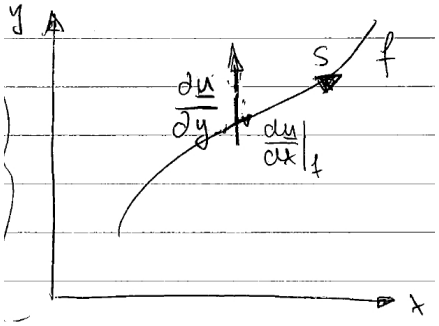


Figure 1.2: Curve $f(x, y)$ with derivatives.

The system (1.2) becomes when eliminating $\frac{\partial \underline{u}}{\partial x}$:

$$\left(\underline{\underline{B}} - \lambda \underline{\underline{A}}\right) \frac{\partial \underline{u}}{\partial y} = -\underline{\underline{A}} \frac{\mathrm{d}\underline{u}}{\mathrm{d}x} + \underline{c} \tag{1.6}$$

with the slope of the curve f

$$\lambda = \left.\frac{\mathrm{d}y}{\mathrm{d}x}\right|_f . \tag{1.7}$$

We look for specific curves f, for which in their neighbourhood the evolution of $\underline{u}$ along f is not sufficient to determine the complete $\underline{u}$, *i.e.* knowing $\left.\frac{\mathrm{d}\underline{u}}{\mathrm{d}x}\right|_f$ is not enough to compute $\frac{\partial \underline{u}}{\partial y}$:

$$\det(\mathrm{B} - \lambda \mathrm{A}) = 0 , \tag{1.8}$$

or λ being an eigenvalue of $\mathrm{B}\underline{a} = \lambda \mathrm{A}\underline{a}$. These specific curves $f(x, y) = 0$ with $\lambda = \frac{\mathrm{d}y}{\mathrm{d}x}$ are called **characteristics** of the system (1.2).

The solution might have discontinuities *across* characteristics. On the other hand, information propagates *along* characteristics. Typically, along characteristics, a simpler equation (reduced order) holds ($\Rightarrow$ method of characteristics).

Definition 1.2 ***Type of partial differential equation*:** Depending on the eigenvalues λ, we call the type of the linear system of PDEs (1.2):

a *hyperbolic* if n real eigenvalues and n linearly independent eigenvectors $\underline{a}$ exist,

b *parabolic* if n real eigenvalues and less than n linearly independent eigenvectors exist,

c *elliptic* if n complex (non-real) eigenvalues exist, or

d *mixed type* if real and complex eigenvalues exist.

□

Example 1.2 ***Prandtl–Glauert equation*****:**

$$(1 - M_\infty^2)\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0 \tag{1.9}$$

This equation describes the 2D, inviscid, linearised, compressible steady flow over a thin (streamlined) body, see Fig. 1.3. M_∞ is the Mach number

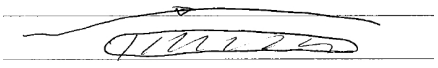


Figure 1.3: Flow over a thin body as considered in the Prandtl–Glauert equation.

$$M_\infty = \frac{u_\infty}{c_\infty} \ , \tag{1.10}$$

with the speed of sound c_∞ and the velocity potential

$$u = \frac{\partial \phi}{\partial x} \qquad v = \frac{\partial \phi}{\partial y} \ . \tag{1.11}$$

One can re-write the original system as

$$\begin{cases} (1 - M_\infty^2)u_x + v_y = 0 \\ u_y - v_x = 0 \ , \end{cases} \tag{1.12}$$

where the second equation comes from $\phi_{xy} = \phi_{yx}$ (equality of mixed partials). In more compact form we get

$$\underline{u} = \begin{pmatrix} u \\ v \end{pmatrix} \qquad A = \begin{pmatrix} 1 - M_\infty^2 & 0 \\ 0 & -1 \end{pmatrix} \qquad B = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \ , \tag{1.13}$$

so that the eigenvalue problem

$$B\underline{a} = \lambda A\underline{a} \tag{1.14}$$

has the solution

$$\lambda_{1,2} = \pm \left(\sqrt{M_\infty^2 - 1} \right)^{-1} \tag{1.15}$$

and

$$\underline{a}_{1/2} = (1, \pm\sqrt{M_\infty^2 - 1}) \ . \tag{1.16}$$

For subsonic flow ($M_\infty < 1$), the type is elliptic as the eigenvalues are complex. For supersonic flow ($M_\infty > 1$), it is hyperbolic as the eigenvalues are real and the eigenvectors distinct. For $M_\infty = 1$ the equation is parabolic.

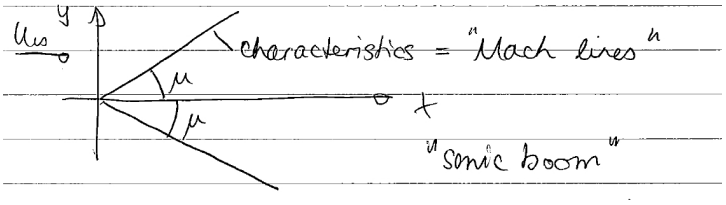


Figure 1.4: Hyperbolic solution to the Prandtl–Glauert equation.

This is an example of an equation that changes type depending on parameters (in this case the Mach number, which could even change locally). Note that the time-dependent problem is always hyperbolic.

In the hyperbolic case, $M_\infty > 1$ and shown in Fig. 1.4, we can define the angle μ as

$$\sin\mu = 1/M_\infty \quad \Rightarrow \quad \lambda_{1/2} = \pm\left(\sqrt{M_\infty^2 - 1}\right)^{-1} = \pm\tan\mu \ . \tag{1.17}$$

These characteristics are also called *Mach lines*. □

Extension: Linear PDE of the second order:

$$E\frac{\partial^2 u}{\partial x^2} + F\frac{\partial^2 u}{\partial x \partial y} + G\frac{\partial^2 u}{\partial y^2} + H = 0 \tag{1.18}$$

with $\lambda = \left.\frac{dy}{dx}\right|_c$:

$$E\lambda^2 - F\lambda + G = 0 \tag{1.19}$$

- *hyperbolic* if two real characteristic:

$$F^2 - 4EG > 0 \tag{1.20}$$

- *parabolic* if one real characteristic:

$$F^2 - 4EG = 0 \tag{1.21}$$

- *elliptic* if complex characteristics:

$$F^2 - 4EG < 0 \tag{1.22}$$

1.3.1 Elliptic equations

Elliptic problems are typically steady diffusion processes, with no marching properties (neither in space nor in time). The most prominent model equations are the Laplace and Poisson equations.

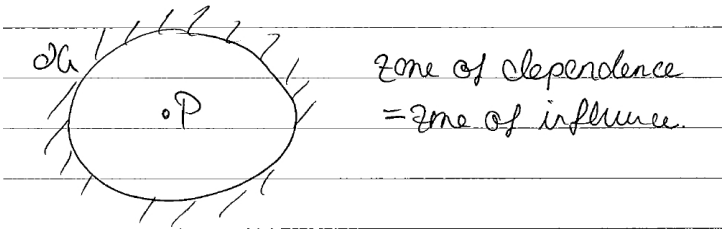


Figure 1.5: Domain and boundaries for an elliptic equation.

Example 1.3 ***Poisson and Laplace equations*** ***($f = 0$)*****:** The typical example for an elliptic equation is the Poisson equation,

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \Delta u = f \ , \tag{1.23}$$

which in the case of $f = 0$ is a Laplace equation. □

For elliptic problems, boundary conditions need to be given at all points of the boundary, as shown in Fig. 1.5. One can distinguish a number of different types of boundary conditions, of which the three most common ones are the following:
Dirichlet boundary condition:

$$u\Big|_{\partial G} = g_1(x, y) \tag{1.24}$$

Neumann boundary condition:

$$\frac{\partial u}{\partial n}\Big|_{\partial G} = g_2(x, y) \tag{1.25}$$

Robin boundary condition:

$$\left(\frac{\partial u}{\partial n} + \alpha u\right)\Big|_{\partial G} = g_3(x, y) \tag{1.26}$$

For elliptic problems, the following observations can be made:

- Compatibility condition in case only Neumann conditions are given: Start with $\Delta u = f$ and integrate over the whole domain:

$$\int_G f \mathrm{d}V = \int_G \Delta u \mathrm{d}V = \int_G \nabla \cdot \nabla u \mathrm{d}V \tag{1.27}$$

  Then one can apply the Gauss theorem

$$\int_G f \mathrm{d}V = \int_{\delta G} \nabla u \cdot n \mathrm{d}S = \int_{\delta G} g_2 \mathrm{d}S \ . \tag{1.28}$$

  So one sees that the forcing f and the boundary condition g_2 need to fulfill specific compatibility conditions in order to allow for a solution. Physically, it expresses that the flux through the boundary needs to be compensated with a source term inside the domain.

- Solution u is smoother that f.
- well-behaved solutions.
- Since we have to solve for all points at the same time $\Rightarrow$ memory consuming (see homework problems).

1.3.2 Hyperbolic problems

Typical examples for hyperbolic equations are the wave equation, advection equation and the compressible Euler equation (transient). Hyperbolic problems describe advection processes with wave-like character, however without dissipation (undamped).

Example 1.4 ***Linear wave equation*****:** The simplest example for a hyperbolic problem is the linear wave equation (also called advection or convection equation),

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0 \ , \tag{1.29}$$

with a real speed c. □

To analyse the behaviour of the solution, consider the following:

$$\begin{cases} \frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0 \\ \frac{\mathrm{d}u}{\mathrm{d}t}\Big|_f = \frac{\partial u}{\partial t} + \frac{\mathrm{d}x}{\mathrm{d}t}\Big|_f \frac{\partial u}{\partial x} \end{cases} \qquad \Rightarrow \quad \frac{\mathrm{d}u}{\mathrm{d}t}\Big|_f = (\lambda - c)\frac{\partial u}{\partial x} \tag{1.30}$$

choose:

$$\frac{\mathrm{d}u}{\mathrm{d}t}\Big|_f = 0 \qquad \lambda = \frac{\mathrm{d}x}{\mathrm{d}t}\Big|_f = c \tag{1.31}$$

Classical wave solution:

$$u = \hat{u}e^{i(kx-\omega t)} \tag{1.32}$$

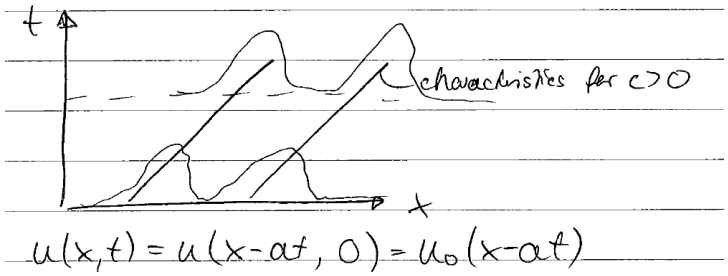


Figure 1.6: Solution to the linear wave equation.

- along curves f with $\mathrm{d}x/\mathrm{d}t|_f = c$ the solution is constant.

- λ is real $\Rightarrow$ hyperbolic problem
- convection of initial data along characteristics
- Well-posedness means that one needs to provide boundary or initial conditions according to the number of *incoming* characteristics (Fig. 1.7).

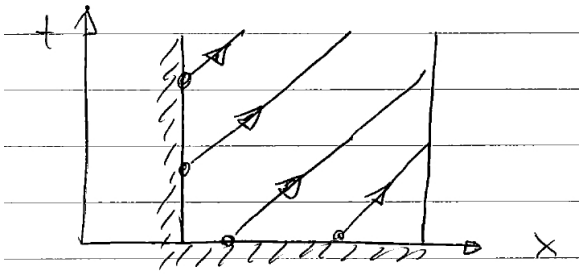


Figure 1.7: Well-posedness: the hatched boundaries need to provide boundary or initial conditions.

Example 1.5 ***Burgers equation*****:**

$$\frac{\partial u}{\partial t} + u \cdot \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2} \tag{1.33}$$

- nonlinear equation (here the one-dimensional viscous Burgers equation in quasi-linear form),
- There is a viscous version and an inviscid version (with $\nu = 0$). For the hyperbolic problem, we consider the inviscid version here.
- speed of the characteristics: $\mathrm{d}x/\mathrm{d}t|_f = u$
- solution along characteristics: $\mathrm{d}u/\mathrm{d}t|_f = 0$, *i.e.* constant.
- might lead to crossing of characteristics $\Rightarrow$ shocks, despite smooth initial conditions, see Fig. 1.8.

□

Example 1.6 ***System with two characteristics per point*****:** Consider a hyperbolic problem with two variables $\underline{u} = (u, v)$ in a space–time (x, t) plane. Then the zone of influence and the region of dependence of a point P are wedges starting in P, as shown in Fig. 1.9. □

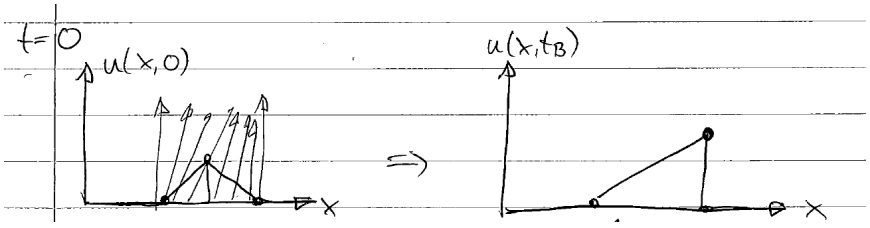


Figure 1.8: Development of a shock for the Burgers equation.

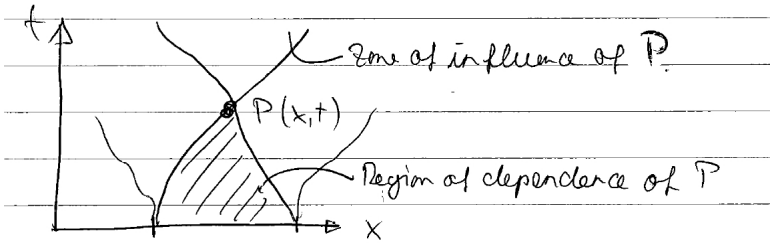


Figure 1.9: Dependency of the function value in P for a hyperbolic problem.

1.3.3 Parabolic equation

The most prominent examples of parabolic equations are the heat (or diffusion) equation. Parabolic problems typically describe the following

- equilibrating processes, time dependent
- smoothing properties, smearing out over time.

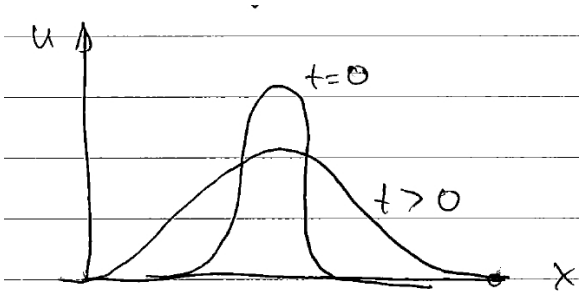


Figure 1.10: Typical behaviour of a parabolic equation.

Example 1.7 ***Heat equation*****:** The typical example for a parabolic equation is the heat (or diffusion) equation, which can be written in one or multiple dimensions. In the 1D case is reads

$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2} \tag{1.34}$$

□

In order to determine the type of the heat equation, we rewrite the equation as a system of two first-order equations,

$$\begin{cases} \frac{\partial u}{\partial t} - \nu \frac{\partial v}{\partial x} = 0 \\ \frac{\partial u}{\partial x} = v \end{cases} \tag{1.35}$$

So:

$$\underline{u} = \begin{pmatrix} u \\ v \end{pmatrix}, \quad A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & -\nu \\ 1 & 0 \end{pmatrix}, \quad c = \begin{pmatrix} 0 \\ v \end{pmatrix} \tag{1.36}$$

the heat equation is parabolic:

$$\det(B - \lambda A) = \det \begin{vmatrix} -\lambda & -\nu \\ 1 & 0 \end{vmatrix} = -\lambda \cdot 0 + \nu = 0 \tag{1.37}$$

because $\lambda = \infty$ is real and the two eigenvectors are the same. The characteristics are thus horizontal in a space–time plot (Fig. 1.11). Boundary conditions need to be given on δZ and initial conditions on G. Note the compatibility between δZ and G.

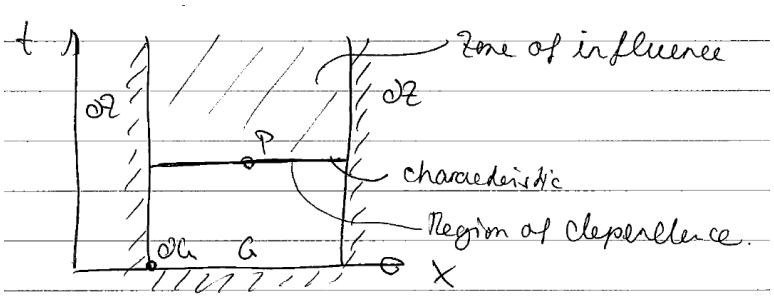


Figure 1.11: Space–time plot of a parabolic equation.

Example 1.8 ***Linear system of equations*****:**

$$\frac{\partial \underline{u}}{\partial t} + \begin{pmatrix} a & b \\ b & a \end{pmatrix} \frac{\partial \underline{u}}{\partial x} = 0 \tag{1.38}$$

$$\underline{u} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}, \quad A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} a & b \\ b & a \end{pmatrix}, \quad \underline{c} = 0 \tag{1.39}$$

Characteristic equation:

$$(B - \lambda A) \frac{\partial \underline{u}}{\partial x} = -A \frac{d\underline{u}}{dt}\Big|_f + \underline{c} \tag{1.40}$$

$$\lambda = \frac{dx}{dt}\Big|_f \tag{1.41}$$

Eigenvalues:

$$B\underline{a} = \lambda\underline{a} \tag{1.42}$$

Hyperbolic case:

$$\underline{a}_{1,2} = \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}, \quad \lambda_{1,2} = a \pm b \tag{1.43}$$

So that:

$$T^{-1} = \begin{pmatrix} \underline{a}_1 & \underline{a}_2 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad \underline{u} = T^{-1}\underline{\omega} \tag{1.44}$$

$$T = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & -1/2 \end{pmatrix} \qquad \underline{\omega} = T\underline{u} \tag{1.45}$$

So that:

$$\frac{\partial \omega}{\partial t} = TBT^{-1}\frac{\partial \omega}{\partial x} = 0 \tag{1.46}$$

$$\frac{\partial \omega_1}{\partial t} + \lambda_1 \frac{\partial \omega_1}{\partial x} = 0 \quad \Rightarrow \quad \frac{dx}{dt} = \lambda_1 \quad \Rightarrow \frac{d\omega_1}{dt} = 0 \tag{1.47}$$

$$\frac{\partial \omega_2}{\partial t} + \lambda_2 \frac{\partial \omega_2}{\partial x} = 0 \quad \Rightarrow \quad \frac{dx}{dt} = \lambda_2 \quad \Rightarrow \frac{d\omega_2}{dt} = 0 \tag{1.48}$$

□

1.4 Main points to remember

⇒ 3 different types of PDE

- hyperbolic: convection and waves
- parabolic: time-dependent diffusion
- elliptic: steady diffusion
- mixed

⇒ Numerical treatment and boundary/initial conditions depend on type.
⇒ Characteristics (hyperbolic problems) transport information.
⇒ Well-posedness.

2 Finite-difference schemes

Finite differences (FD):

- the dependent variables, $u(x,t)$, are considered to exist at discrete grid points, leading to grid functions, *e.g.:* $u_{i,j} = u(x_i, y_j)$, $u^n_j = u(x_j, t^n)$, *etc.*;
- derivatives are approximated by differences, leading to an algebraic representation of the PDEs.

In case of equidistant grid points (not necessary, in general)

$$\Delta x = \frac{L_x}{N_x - 1} \qquad \Delta y = \frac{L_y}{N_y - 1}, \tag{2.1}$$

where L_x and L_y are the domain size and N_x and N_y the number of grid points in the two directions. This then defines the so-called grid function

$$u_{ij} = u(x_i, y_j) \ .$$

The discretisation in time (Chapter 3) is typically added as a superscript

$$u^n_j = u(x_j, t^n) \ .$$

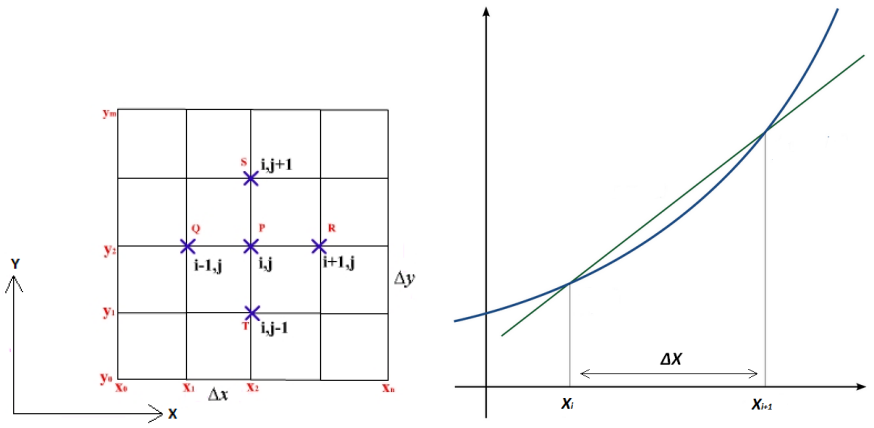


Figure 2.1: (Left) Example of a finite difference approximation on a 2D equidistant grid and (right) first order approximation.

2.1 Derivation of finite difference schemes

General principle: Use Taylor series, and cancel error terms up to a specific order.

$$u(x+\Delta x) = u(x) + \Delta x \frac{\partial u}{\partial x} + \frac{1}{2!}\Delta x^2 \frac{\partial^2 u}{\partial x^2} + \frac{1}{3!}\Delta x^3 \frac{\partial^3 u}{\partial x^3} + ... \tag{2.2}$$

$$\frac{\partial u}{\partial x} = \frac{u(x+\Delta x) - u(x)}{\Delta x} - \frac{1}{2}\Delta x \frac{\partial^2 u}{\partial x^2} + \mathcal{O}(\Delta x^2) \tag{2.3}$$

which can be written as a matrix-vector product:

$$\underline{u}_N = \begin{pmatrix} \cdots \\ u_{i-1} \\ u_i \\ u_{i+1} \\ \cdots \end{pmatrix}, \quad D_+^N = \frac{1}{\Delta x} \begin{pmatrix} \cdots & \cdots & & & \\ & -1 & 1 & & \\ & & -1 & 1 & \\ & & & \cdots & \cdots \end{pmatrix} \quad \Rightarrow \quad \underline{u}'_N \simeq D_+^N \cdot \underline{u}_N \tag{2.4}$$

Central difference (second order):

$$D_0 u_i = \frac{u_{i+1} - u_{i-1}}{2\Delta x} = u'(x_i) + \mathcal{O}(\Delta x^2) \tag{2.5}$$

Backward/left-sided difference (first order):

$$D_- u_i = \frac{u_i - u_{i-1}}{\Delta x} = u'(x_i) + \mathcal{O}(\Delta x) \tag{2.6}$$

Forward/right-sided difference (first order):

$$D_+ u_i = \frac{u_{i+1} - u_i}{\Delta x} = u'(x_i) + \mathcal{O}(\Delta x) \tag{2.7}$$

2.2 Truncation error

The truncation error is the difference between the numerical and exact derivative, and due to selecting a number of discrete points in space with a finite spacing, *i.e.* grid spacing $\Delta x > 0$. Using Taylor expansion:

$$D_0 u_i - u' \Big|_{x_i} = \frac{u(x_i + \Delta x) - u(x_i - \Delta x)}{2\Delta x} - \frac{\mathrm{d}u}{\mathrm{d}x}\Big|_{x_i} \tag{2.8}$$

$$D_0 u_i - u' \Big|_{x_i} = \frac{1}{6}\Delta x^2 \frac{\mathrm{d}^3 u}{\mathrm{d}x^3}\Big|_{x_i} + \cdots = \mathcal{O}(\Delta x^2)\ . \tag{2.9}$$

In this case, the leading error term is $\mathcal{O}(\Delta x^2)$, therefore D_0 is called finite differences of *second* order. Important: The error goes to zero for $\Delta x \to 0$.

2.3 Modified wavenumber

With a Taylor expansion we performed a local analysis in terms of the grid spacing. The concept of the modified wavenumber allows to perform a global analysis in terms of wave numbers.

Consider a function periodic on $L = 2\pi$.

$$u(x) = e^{ikx} \tag{2.10}$$

$$e^{i\phi} = \cos\phi + i\sin\phi \tag{2.11}$$

Exact derivative for a Fourier mode:

$$u'(x)_{\text{exact}} = ike^{ikx} \tag{2.12}$$

Using a finite difference schemes:

$$u'(x)_{\text{num}} = i\tilde{k}e^{ikx} \quad \Rightarrow \quad \tilde{k}(k) = \frac{u'(x)_{\text{num}}}{ie^{ikx}} \tag{2.13}$$

The exact modified wavenumber would be $\tilde{k} = k$. Any departure from from that is a measure of the global accuracy of the chosen scheme, as a function of wavenumber k, *i.e.* the scale (or wavelength) of the derivative considered.

Example 2.1 ***Central difference scheme*:**

$$u'(x)_{\text{num}} = \frac{u(x+\Delta x) - u(x-\Delta x)}{2\Delta x} = \frac{1}{2\Delta x}\left(e^{ik(x+\Delta x)} - e^{ik(x-\Delta x)}\right) \tag{2.14}$$

$$u'(x)_{\text{num}} = i\frac{\sin(k\Delta x)}{\Delta x}e^{ikx} = i\tilde{k}e^{ikx} \tag{2.15}$$

so:

$$\tilde{k}(k)\Delta x = \sin(k\Delta x)\,, \quad k = 0, \ldots, \frac{N}{2} \tag{2.16}$$

As shown in Fig. 2.2b, for long wavelengths (region A) the approximation D_0 is good, however for short waves (region B), increased damping of the derivative is observed. Note: for asymmetric schemes, the modified wavenumber is complex, leading not only to amplitude errors but also to phase errors (lagging of waves) in the derivative. □

2.4 Table: Finite difference formulas for first derivatives

Left-sided finite difference scheme first order:

$$\left.\frac{\partial u}{\partial x}\right|_{x_i} = \frac{u_i - u_{i-1}}{\Delta x} + \frac{\Delta x}{2}\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} + \ldots \tag{2.17}$$

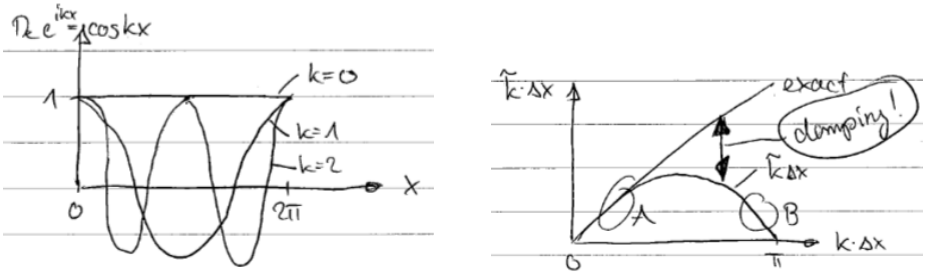


Figure 2.2: (Left) Fourier decomposition of a certain function (right) modified wave-number.

Left-sided finite difference scheme second order:

$$\left.\frac{\partial u}{\partial x}\right|_{x_i} = \frac{3u_i - 4u_{i-1} + u_{i-2}}{2\Delta x} + \frac{\Delta x^2}{3}\left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \dots \tag{2.18}$$

Right-sided finite difference scheme first order:

$$\left.\frac{\partial u}{\partial x}\right|_{x_i} = \frac{u_{i+1} - u_i}{\Delta x} - \frac{\Delta x}{2}\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} + \dots \tag{2.19}$$

Right-sided finite difference scheme second order:

$$\left.\frac{\partial u}{\partial x}\right|_{x_i} = \frac{-3u_i + 4u_{i+1} - u_{i+2}}{2\Delta x} + \frac{\Delta x^2}{3}\left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \dots \tag{2.20}$$

Central finite difference scheme second order:

$$\left.\frac{\partial u}{\partial x}\right|_{x_i} = \frac{u_{i+1} - u_{i-1}}{2\Delta x} - \frac{\Delta x^2}{6}\left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \dots \tag{2.21}$$

Central finite difference scheme fourth order:

$$\left.\frac{\partial u}{\partial x}\right|_{x_i} = \frac{-u_{i+2} + 8u_{i+1} - 8u_{i-1} + u_{i-2}}{12\Delta x} + \frac{\Delta x^4}{30}\left.\frac{\partial^5 u}{\partial x^5}\right|_{x_i} + \dots \tag{2.22}$$

2.5 Table: Finite difference formulas for second derivatives

Left-sided finite difference scheme first order:

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} = \frac{u_i - 2u_{i-1} + u_{i-2}}{\Delta x^2} + \Delta x\left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \dots \tag{2.23}$$

Left-sided finite difference scheme second order:

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} = \frac{2u_i - 5u_{i-1} + 4u_{i-2} - u_{i-3}}{\Delta x^2} - \frac{11\Delta x^2}{12}\left.\frac{\partial^4 u}{\partial x^4}\right|_{x_i} + \dots \tag{2.24}$$

Right-sided finite difference scheme first order:

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} = \frac{u_{i+2} - 2u_{i+1} + u_i}{\Delta x^2} - \Delta x \left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \dots \tag{2.25}$$

Right-sided finite difference scheme second order:

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} = \frac{2u_i - 5u_{i+1} + 4u_{i+2} - u_{i+3}}{\Delta x^2} + \frac{11\Delta x^2}{12} \left.\frac{\partial^4 u}{\partial x^4}\right|_{x_i} + \dots \tag{2.26}$$

Central finite difference scheme second order:

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} - \frac{\Delta x^2}{12} \left.\frac{\partial^4 u}{\partial x^4}\right|_{x_i} + \dots \tag{2.27}$$

Central finite difference scheme fourth order:

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} = \frac{-u_{i+2} + 16u_{i+1} - 30u_i + 16u_{i-1} - u_{i-2}}{12\Delta x^2} + \frac{\Delta x^4}{90} \left.\frac{\partial^6 u}{\partial x^6}\right|_{x_i} + \dots \tag{2.28}$$

2.6 Table: Finite difference formulas for third derivatives

Central finite difference scheme second order:

$$\left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} = \frac{u_{i+2} - 2u_{i+1} + 2u_{i-1} - u_{i-2}}{2\Delta x^3} - \frac{\Delta x^2}{4} \left.\frac{\partial^5 u}{\partial x^5}\right|_{x_i} + \dots \tag{2.29}$$

Central finite difference scheme fourth order:

$$\left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} = \frac{-u_{i+3} + 8u_{i+2} - 13u_{i+1} + 13u_{i-1} - 8u_{i-2} + u_{i-3}}{8\Delta x^3} + \frac{7\Delta x^4}{120} \left.\frac{\partial^7 u}{\partial x^7}\right|_{x_i} + \dots \tag{2.30}$$

2.7 Table: Finite difference formulas for fourth derivatives

Central finite difference scheme second order:

$$\left.\frac{\partial^4 u}{\partial x^4}\right|_{x_i} = \frac{u_{i+2} - 4u_{i+1} + 6u_i - 4u_{i-1} + u_{i-2}}{\Delta x^4} - \frac{\Delta x^2}{6} \left.\frac{\partial^6 u}{\partial x^6}\right|_{x_i} + \dots \tag{2.31}$$

3 Discretisation in time

So far we have considered the discretisation in space:

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0 \qquad \frac{\partial u}{\partial x}\Big|_i \approx \frac{u_i - u_{i-1}}{\Delta x} + \mathcal{O}(\Delta x) \tag{3.1}$$

Semidiscretization:

$$\frac{\partial u}{\partial t} = L(u) = -\frac{\partial u}{\partial x} \quad \Rightarrow \quad \frac{\mathrm{d}u_i}{\mathrm{d}t} = L_N(u_i) \tag{3.2}$$

We have a transformation of the original PDE to an ODE of the grid function.

3.1 Euler method

Now we need to find methods to integrate an ODE of the form $\mathrm{d}u_i/\mathrm{d}t = L_N(u_i)$. The most straightforward way is to use first-order finite differences in time: the so-called Euler method.

$$\frac{du_i}{dt} \approx \frac{u_i^{n+1} - u_i^n}{\Delta t} + \mathcal{O}(\Delta t) \ . \tag{3.3}$$

Note that the superscripts n and $n+1$ denote the time level. The question is when to evaluate L_N, which gives two variants:

- Euler forward:
$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = L_N(u_i^n) \tag{3.4}$$
- Euler backward:
$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = L_N(u_i^{n+1}) \tag{3.5}$$

The difference is that the right-hand side (RHS) is evaluated at either the old time step t^n or the new time step t^{n+1}.

Example 3.1 ***Advection equation*:** Euler forward (forward time backward space – FTBS), **explicit**:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -\frac{u_i^n - u_{i-1}^n}{\Delta x} = -D_- u_i^n \quad \Rightarrow \quad u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x}(u_i^n - u_{i-1}^n) \tag{3.6}$$

- one equation per grid point
- easy to implement, very straight-forward
- However, usually restriction on time step size Δt

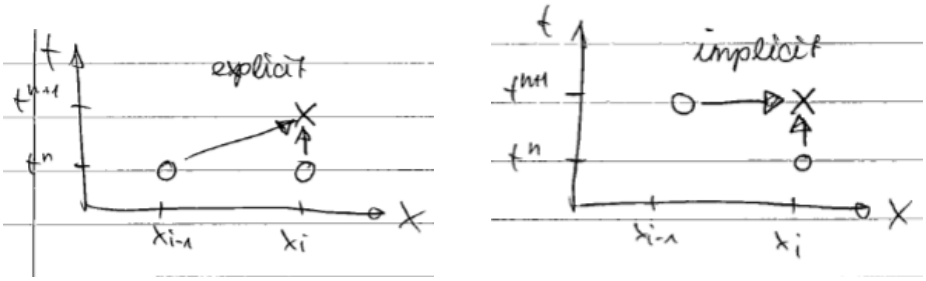


Figure 3.1: Graphical representation of the (right) explicit and (left) implicit Euler method in a space–time plane.

Euler backward (backward time backward space – BTBS), **implicit**:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -\frac{u_i^{n+1} - u_{i-1}^{n+1}}{\Delta x} = -D_- u_i^{n+1} \quad \Rightarrow \quad (1 + \Delta t D_-) u_i^{n+1} = u_i^n \tag{3.7}$$

- For each time step, we have to solve an equation system:

$$A u_i^{n+1} = u_i^n \tag{3.8}$$

- It is more difficult to implement, and it has larger memory requirements, which scales as $N^D \times N^D$, where N and D are the number of grid points and the dimensions of the problem, respectively.
- It has larger stability bounds.

□

Other popular time-integration methods are:

- Crank–Nicolson: it is a combination of explicit and implicit Euler, giving order Δt^2 (see HW2).
- Runge-Kutta (RK) with substeps (HW3),
- multi-steps methods, *e.g.:* Adams–Bashforth (explicit) and Adam–Moulton (implicit).

Some of these methods will be used in the homeworks. Note that for instance Matlab and Python include implementations of these integration schemes.

3.2 Characteristic polynomial

The amplification factor $G(z)$ defines the characteristic polynomial for the various integration schemes, as well as the exact integration of the Dahlquist equation. With $z = \lambda \Delta z$ one gets

- explicit Euler method:

$$G(z) = \frac{u^{n+1}}{u^n} = 1 + z \tag{3.9}$$

- implicit Euler method:

$$G(z) = \frac{1}{1 - z} \tag{3.10}$$

- Crank–Nicolson method:

$$G(z) = \frac{1 + z/2}{1 - z/2} \tag{3.11}$$

- exact:

$$G(z) = e^z \tag{3.12}$$

One can see that the charactersitic polynomials for the different integration methods are essentially rational approximation of the exponential e^z around $z = 0$, as illustrated in Fig. 3.2. It becomes also obvious that the behaviour of

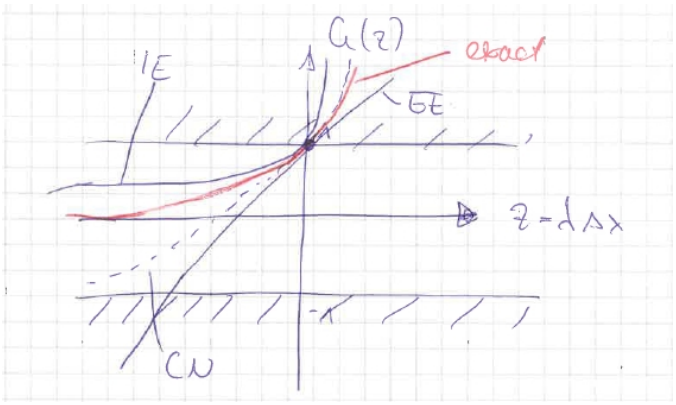


Figure 3.2: Characteristic polynomial for various approximations $G(z)$ with real $z = \lambda\Delta x$: explicit Euler (EE), implicit Euler (IE), Crank–Nicolson (CN). The hatched area indicates the region where the schemes are unstable.

the different schemes differs as $z \to -\infty$. Such problems are typically called stiff problems as they are related to very fast time scales (large negative z). The explicit Euler scheme diverges towards minus infinity, which shows that it is, as shown above, unstable for large negative z. The Crank–Nicolson scheme goes to -1, and the implicit Euler scheme to 0, as does the exact solution. This shows that CN tends to give stable (*i.e.* non growing) but oscillating results, which is not the case for the implicit Euler scheme which will converge monotonically.

In this context, two expressions can be defined: An integration scheme is called

- A-stable if $|G| \leq 1$ for all $\lambda \leq 0$,
- and L-stable if in addition $\lim_{z\to-\infty} G(z) = 0$.

The latter schemes are best suited for stiff problems.

3.3 Table: Finite differences for the integration of ODEs

Ordinary differential equation:

$$\frac{\mathrm{d}u}{\mathrm{d}t} = f(u,t),\ u^n = u(t^n),\ f^n = (u^n, t^n),\ t^n = n\Delta t \tag{3.13}$$

Explicit Euler scheme, order $\mathcal{O}(\Delta t)$:

$$u^{n+1} = u^n + \Delta t \cdot f^n \tag{3.14}$$

Implicit Euler scheme, order $\mathcal{O}(\Delta t)$:

$$u^{n+1} = u^n + \Delta t \cdot f^{n+1} \tag{3.15}$$

(Generalised) Crank-Nicolson scheme:

$$u^{n+1} = u^n + \Delta t([1-\theta]\cdot f^n + [\theta]\cdot f^{n+1})\ ,\quad 0 \leq \theta \leq 1 \tag{3.16}$$

[The standard Crank–Nicolson scheme is given by $\theta = 0.5$ with order $\mathcal{O}(\Delta t^2)$; the explicit and implict Euler schemes are obtained with $\theta = 0$ and $\theta = 1$, respectively.]
Standard Runge–Kutta scheme (RK4), order $\mathcal{O}(\Delta t^4)$:

$$u^{n+1} = u^n + \frac{\Delta t}{6}(f^n + 2k_1 + 2k_2 + k_3) \tag{3.17}$$

$$\text{with}: \quad u_1 = u^n + \frac{\Delta t}{2} f^n,\ k_1 = f(u_1, t^{n+\frac{1}{2}}),\ t^{n+\frac{1}{2}} = t^n + \frac{\Delta t}{2} \tag{3.18}$$

$$u_2 = u^n + \frac{\Delta t}{2} k_1,\ k_2 = f(u_2, t^{n+\frac{1}{2}}) \tag{3.19}$$

$$u_3 = u^n + \Delta t k_2,\ k_3 = f(u_3, t^{n+1}) \tag{3.20}$$

3.4 Points to remember

Finite differences:

- approximation of derivatives via Taylor expansion;
- modified wavenumber: global (spectral) analysis;
- semidiscretisation: PDE transformed to ODE.
- time discretisation: explicit & implicit.

4 Analysis of the discretised equations

Summary:

- Physical model ⇒ PDE.
- Classify PDE ⇒ expected behaviour.
- Choose discretisation ⇒ FD, however
  - central differences / skewed differences;
  - time integration (explicit, implicit).

  Can we choose any discretisation? NO!

Now, analysis of the discretised system:

1. Consistency — order of accuracy;
2. Stability — von Neumann analysis, modified differential equation;
3. Convergence — Lax–Richtmyer (LR) equivalence theorem;

To answer the questions:

1. How well do we approximate the PDE?
2. Sensitivity to disturbances, *i.e.* will the solution blow up at some time?
3. Do we really approximate a true (correct) solution?

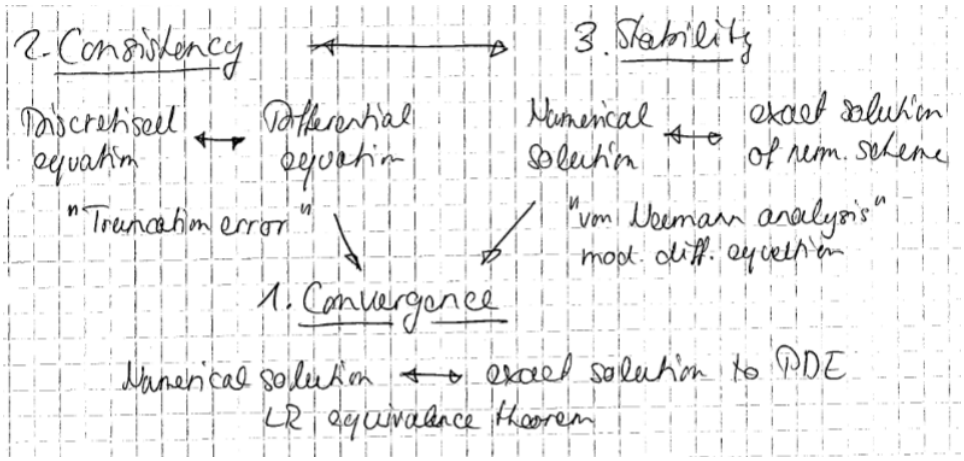


Figure 4.1: Schematic representation of the concepts of consistency, stability and convergence.

4.1 Convergence

Does the numerical solution approach the exact solution as the mesh is refined?

Definition 4.1 ***Convergence*:**

$$||u_j^n - u(x_j, y^n)|| \leq C(\Delta x^p + \Delta t^q), \text{ for } \Delta x,\ \Delta t \to 0, \text{with} p, q, C > 0 \quad (4.1)$$

where p and q are the rate of convergence. □

It is very difficult to show convergence without knowing the exact solution, however we can use a theorem by Lax and Richtmyer: *Given a linear, well-posed initial value problem, if the FD approximation is* ***consistent*** *and* ***stable****, convergence is assured (necessary and sufficient condition).*

$$\begin{cases} \text{Consistency: } \lim\limits_{\Delta x, \Delta t \to 0} T \to 0 \\ \text{Stability: } |G| < 1 \end{cases} \quad \Leftrightarrow \quad \text{Convergence: } \lim_{\Delta x, \Delta t \to 0} u_j^n \to u(x_j, t^n) \quad (4.2)$$

Therefore, it is important to discuss the concepts of consistency (Section 4.2) and stability (Section 4.3).

4.2 Consistency

Consistency essentially means how well we approximate the PDE.

$$\text{PDE: } P(x, t, \partial_x, \partial_t)[u] = f,\ u(x, 0) = g \quad (4.3)$$

$$\text{discrete: } P_N(x, t, \Delta x, \Delta t)[u_n] = f_N,\ u_N(x, 0) = g_N \quad (4.4)$$

Therefore, one defines the truncation error as the difference between exact PD and its discrete representation:

Definition 4.2 ***Local truncation error*:**

$$T(x_j, t^n) = P[v]_{x_j, t^n} - P_N[v_N]_{x_j, t^n} \quad (4.5)$$

□

Consistency now means that this error needs to go to zero for smaller and smaller grid spacings in space and time.

Definition 4.3 ***Consistency*:**

$$||T(x_j, t^n)|| \leq C(t^n)(\Delta x^p + \Delta t^q) \text{ with: } C,\ p,\ q > 0$$

where p and q are called the (consistency) order of the spatial and temporal discretization, respectively. □

Example 4.1 ***Advection equation*****:**

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \tag{4.6}$$

FTBS (forward time, backward space):

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\frac{u_j^n - u_{j-1}^n}{\Delta x} = 0 \tag{4.7}$$

Idea: Use Taylor expansion:

$$\begin{aligned} u_j^{n+1} &= u(x_j, t^n) + \Delta t u_t + \frac{1}{2}\Delta t^2 u_{tt} + \mathcal{O}(\Delta t^3) \\ u_{j-1}^n &= u(x_j, t^n) - \Delta x u_x + \frac{1}{2}\Delta x^2 u_{xx} + \mathcal{O}(\Delta x^3) \end{aligned} \tag{4.8}$$

Substituting equation (4.8) into (4.7):

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = -\frac{1}{2}\Delta t u_{tt} + a\frac{1}{2}\Delta x u_{xx} + \mathcal{O}(\Delta t^2) + \mathcal{O}(\Delta x^2) \tag{4.9}$$

Using (4.5) to get the truncation error

$$T(x_j, t^n) = -\underbrace{\frac{1}{2}\Delta t\, u_{tt}}_{q=1} + \underbrace{\frac{1}{2}a \cdot \Delta x\, u_{xx}}_{p=1} + \mathcal{O}(\Delta t^2, \Delta x^2)\ . \tag{4.10}$$

The truncation error is order one in time and space (order of accuracy). Therefore, the above discretisation is indeed consistent. Using the PDE to relate u_{tt} and u_{xx} (equality of mixed partials):

$$u_{tt} = a^2 u_{xx} \text{ and } \sigma = \frac{a\Delta t}{\Delta x} \quad \Rightarrow \quad T(x_j, t^n) = \frac{1}{2}a\Delta x(1-\sigma)u_{xx} \tag{4.11}$$

□

Example 4.2 ***DuFort–Frankel scheme*****:** There are schemes that are so-called conditionally stable, as *e.g.* the DuFort–Frankel scheme applied to the diffusion equation. In this case, a condition relating both the grid spacing Δx and the time step Δt arises due to consistency, rather than due to stability as for most other cases (note that the DuFort–Frankel scheme is unconditionally stable). □

4.3 Stability

A stable numerical scheme is a scheme for which errors from any source (round off and truncation) are not permitted to grow as the calculation proceeds from one time (or marching) step to the next. In short: the errors must not amplify.

Consider the scheme $P_N[u_N] = 0$ (as before). Write it in the following explicit form

$$u_N^{n+1} = G(\Delta x, \Delta t) u_N^n, \text{with initial condition: } u_N^0 \tag{4.12}$$

Starting from time $t = 0$, we can write

$$u_N^n = G u_N^{n-1} = G(G(u_N^{n-2})) = \cdots = G^n u_N^0 \ . \tag{4.13}$$

Due to linearity, the errors $u_N + \varepsilon$ fulfill the same discretised equation, thereby being amplified with the same operator G:

$$P_N(\varepsilon) = 0 \quad \Rightarrow \quad \varepsilon_N^n = G^n \varepsilon_N^0 \tag{4.14}$$

G is called amplification factor/matrix for the proper discretisation.

Therefore, in order to make sure that errors ε do not amplify, stability means that $||G|| \leq 1$.

4.3.1 Absolute stability for an ODE

Let us consider the Dahlquist equation (see HW2):

$$u' = \lambda u, \quad \lambda \in \mathbb{C} = \lambda_r + i\lambda_i \tag{4.15}$$

This equation has the exact solution:

$$u(t) = Ae^{\lambda t} \tag{4.16}$$

If we define "stability" of a scheme as "u should not grow", the exact solution is stable for $\lambda_r = Re(\lambda) \leq 0$, *i.e.* the left halfplane of the complex $z = \lambda \Delta t$ plane. Let us apply the Euler forward integration scheme,

$$\frac{u^{n+1} - u^n}{\Delta t} = \lambda u^n \quad \Rightarrow \quad u^{n+1} = \underbrace{(1 + \lambda \Delta t)}_{G(\Delta t \cdot \lambda)} u^n \tag{4.17}$$

Stability now means $|G| \leq 1$, *i.e.* the solution does not increase from one time step to another. Using $z = \lambda \Delta t$, then

$$|G| \leq 1 \quad \Leftrightarrow \quad |1 + \lambda \Delta t| = |1 + z| \leq 1 \, , \tag{4.18}$$

which is the description of a circle in the complex z-plane with radius 1 and origin at -1, as shown in Fig. 4.2. The integration of (4.15) via (4.17) is stable if $z = \lambda \Delta t$ is within the hatched area in Fig. 4.2. Compare this to the analytical region of stability (not A-stable).

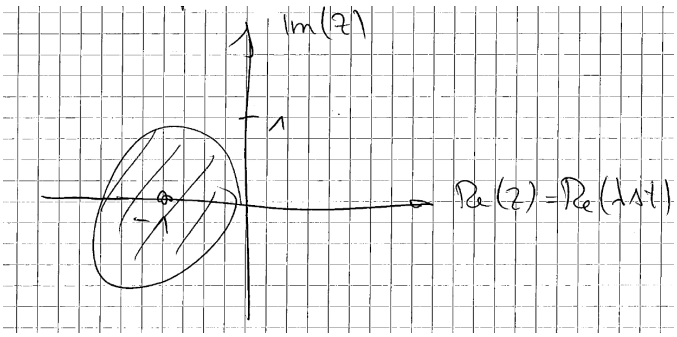


Figure 4.2: Region of absolute stability in the complex $z = \lambda\Delta t$ plane for the forward Euler scheme.

Definition 4.4 *A-stable*: A scheme is *A-stable* if the complete half plane $Re(\lambda\Delta t) < 0$ is contained in the region of absolute stability. □

This definition goes back to Dahlquist (1963). Based on our results we can thus state that:

- The explicit Euler is **NOT** A-stable, therefore restrictions on the time step Δt need to be imposed. This is typical for explicit methods.
- The implicit Euler is A-stable (derivation similar as above). Also that is a typical behaviour for implicit methods.

This is also what was already discussed further above in the context of the characteristic polynomial, see Sec. 3.2 and Fig. 3.2. There also the definition of *L-stable* was introduced.

The computation of the stability bounds for single step schemes can always be done as shown for the example above; this includes also more complicated schemes such as Runge–Kutta schemes. In the case of multi-step schemes one just realises that $u^{n+1} = Gu^n = G^2u^{n-1}$, and will end up with a quadratic (or even higher order) equation. The stability limit is then composed of the minimum $\lambda\Delta t$ for each root.

4.3.2 Von Neumann analysis for PDEs

Going back to John Crank and Phyllis Nicolson (1947) and Jule Charney, Ragnar Fjørtoft and John von Neumann (1950).

- Idea: use a discrete Fourier transform of the solution and consider an individual mode,
- Restrictions: in principle, only applicable to linear PDE with constant coefficient and periodic boundary conditions.

The ansatz for the solution is:

$$u_j^n = \sum_{k=-N/2}^{N/2} \hat{u}_k^n \, e^{ikx_j} \ , \tag{4.19}$$

note the separation of time and space. We consider an individual mode, $\hat{u}_k^n \, e^{ikx_j} = u_j^n$, and we make a substitution in the discretised form in order to compute the amplification factor *per* wavenumber,

$$\hat{G}(k) = \frac{\hat{u}_k^{n+1}}{\hat{u}_k^n} \ . \tag{4.20}$$

The condition for stability in this case becomes

$$\max_k |\hat{G}(k)| \leq 1 + \mathcal{O}(\Delta t) \tag{4.21}$$

Example 4.3 ***Advection equation*:** Discretise the advection equation with FTBS

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a \frac{u_j^n - u_{j-1}^n}{\Delta x} = 0 \, , \tag{4.22}$$

where

$$\begin{aligned} u_j^n &= \hat{u}_k^n e^{ikx_j} \\ u_j^{n+1} &= \hat{u}_k^{n+1} e^{ikx_j} \\ u_{j-1}^n &= \hat{u}_k^n e^{ikx_{j-1}} = \hat{u}_k^n e^{ikx_j} e^{-ik\Delta x} = u_j^n e^{-ik\Delta x} \end{aligned} \tag{4.23}$$

Thus:

$$\hat{u}_k^{n+1} = \left(1 - \underbrace{\frac{\Delta t}{\Delta x} a}_{\sigma} \left(1 - e^{-ik\Delta x} \right) \right) \hat{u}_k^n = \hat{G}(k) \hat{u}_k^n \tag{4.24}$$

$$\hat{G}(k) = \frac{\hat{u}_k^{n+1}}{\hat{u}_k^n} = 1 - \sigma \left(1 - e^{-ik\Delta x} \right) = 1 - \sigma + \sigma e^{ik\Delta x} \tag{4.25}$$

For stability, $|\hat{G}(k)| \leq 1$, which corresponds to require that the circle $\hat{G}$ in the complex plane lays within the circle $|z| = 1$. In the stability limit:

$$\sigma \leq 1 \quad \Rightarrow \quad \frac{a\Delta t}{\Delta x} \leq 1 \tag{4.26}$$

□

This is the so-called CFL condition, named after Courant, Friedrichs, Levy (1920), which is particular relevant for convectively dominated problems, and the so-called *Courant number*

$$\sigma = \frac{a\Delta t}{\Delta x} \ . \tag{4.27}$$

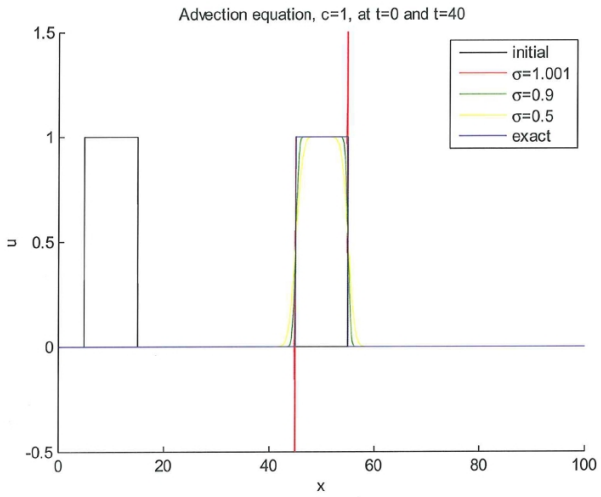


Figure 4.3: Integration of the advection equation, starting with a top-hat initial condition, for different values of the Courant number σ.

For the present discretisation FTBS, in order to have a stable numerical scheme, we need to choose

$$\Delta t \leq \frac{\Delta x}{a} \ . \tag{4.28}$$

An example of how stable and unstable integration may look like in a simulation is given in Fig. 4.3. It can be see that for $\sigma \leq 1$ the initial condition is transported to the right, without overshoots, but increased smoothing for lower σ. However, even a slight increase of σ beyond unity leads to strong growth of the solution, and wiggles at both ends of the square wave.

Example 4.4 ***Negative speed*:** Same as before, but with negative convection velocity, $a < 0$. We get exactly the same $\hat{G} = 1 - \sigma(1 - e^{-ik\Delta x})$ with negative $\sigma = a\Delta t/\Delta x$. However, $1 - \sigma > 1$, so the circle will be outside $|z| = 1$:

- we cannot find a combination of Δx, $\Delta t > 0$ that yields stability;
- therefore the scheme is *unconditionally unstable*.

□

4.3.3 Method of lines

The method of lines typically refers to analysing the properties (in particular also the stability) of schemes by first performing a semi-discretisation to remove the spatial derivatives, and then assessing the temporal stability based on the respective spatial difference operators. In this way, we can

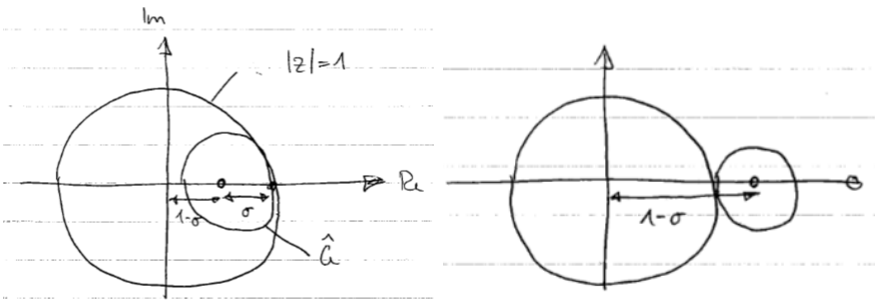


Figure 4.4: Plot of the stability region for the convection equation, left with positive convection velocity, right with negative velocity.

now compare and combine the methods to assess stability introduced in Sections 4.3.1 and 4.3.2.

Consider again the advection equation

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \Rightarrow \frac{\partial u}{\partial t} = L(u) = -a\frac{\partial u}{\partial x} \ . \tag{4.29}$$

The spatial derivatives can now be discretised yielding the semi-discretisation, in this case using one-sided finite differences,

$$\frac{\mathrm{d}u_j}{\mathrm{d}t} = L_N(u_j) = -a\frac{u_j - u_{j-1}}{\Delta x} \ . \tag{4.30}$$

As for the von-Neumann analysis, we make a Fourier ansatz $u_j = \hat{u}_k e^{ix_j k}$, and can thus rewrite equation (4.30) in Fourier space

$$\frac{\mathrm{d}\hat{u}_k}{\mathrm{d}t} = -a\frac{\hat{u}_k - \hat{u}_k e^{-ik\Delta x}}{\Delta x} = \lambda \hat{u}_k \ . \tag{4.31}$$

The last equation sign defines the λ that corresponds to the specific spatial discretisation that needs to be integrated in time,

$$\lambda = \frac{a}{\Delta x}\left(e^{-ik\Delta x} - 1\right) \ . \tag{4.32}$$

Note that equation (4.31) can also be derived using the modified wavenumber pertaining to the specific spatial discretisation. In the present case, we start with the Fourier-transformed advection equation,

$$\frac{\mathrm{d}\hat{u}_k}{\mathrm{d}t} = -a\hat{u}_{k,x} = -ai\tilde{k}\hat{u}_k \ . \tag{4.33}$$

The modified wavenumber $\tilde{k}$ can be derived for the upwind scheme as

$$i\tilde{k}\Delta x = 1 - \cos(k\Delta x) + i\sin(\Delta x) = 1 - e^{-ik\Delta x} \ , \tag{4.34}$$

which is complex as expected for one-sided schemes.

The λ from equation (4.32) describes a circle with centre $-a/\Delta x$ and radius $a/\Delta x$. This λ, for a specific choice of Δx and Δt needs to be contained within the region of absolute stability of the chosen time-integration scheme. For instance, when using the explicit Euler scheme, one can see that the circle from the spatial discretisation and the stability limit from the Euler scheme coincide if $\lambda\Delta t = \lambda\Delta x/a$. This gives the condition for stability $\Delta t \leq \Delta x/a$, which of course is consistent with all the other ways of determining stability.

4.3.4 Method of modified differential equation

The method of modified differential equation is another intuitive approach to assess stability: let us go back to the example of the truncation error. For FTBS:

$$T(x_j, t^n) = \frac{1}{2}a\Delta x(1-\sigma)u_{xx} \tag{4.35}$$

The original PDE is

$$u_t + au_x = 0 \ . \tag{4.36}$$

The discretised version ("modified" PDE) is

$$u_t + au_x = \frac{1}{2}a\Delta x(1-\sigma)u_{xx} + \mathcal{O}(\Delta x^2, \Delta t^2) \ . \tag{4.37}$$

The first term on the right hand side is a diffusive term, with numerical diffusivity, ν_{num} equal to

$$\nu_{\text{num}} = \frac{1}{2}a\Delta x(1-\sigma) \ . \tag{4.38}$$

Since $a > 0 \Rightarrow \nu_{\text{num}} > 0$, thus:

$$1 - \sigma > 0 \quad \Rightarrow \quad \sigma < 1 \ . \tag{4.39}$$

It essentially means that stability for FTBS requires positive numerical viscosity.

4.4 Points to remember

We discussed the convergence of equation:

$$u_t + au_{xx} = 0 \tag{4.40}$$

discretised by FTBS

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{a(u_j^n - u_{j-1}^n)}{\Delta x} = 0 \tag{4.41}$$

We showed that FTBS is

- the system is well-posed (see Lecture 1);
- the discretization is consistent:

$$\lim_{\Delta x,\Delta t\to 0} T = \lim \frac{1}{2} a\Delta x(1-\sigma)u_{xx} = 0 \tag{4.42}$$

- the system is stable for:

$$\sigma = a\frac{\Delta x}{\Delta t} \leq 1 \tag{4.43}$$

Therefore, with the Lax-Richtmyer theorem, the numerical solution that we obtain is indeed converging towards the exact solution when Δx, $\Delta t \to 0$:

$$\lim_{\Delta x,\, \Delta t\to 0} u_j^n \to u(x_j, t^n) \tag{4.44}$$

- Consistency $\Rightarrow$ order of accuracy, truncation error.
- Stability $\Rightarrow$ no error amplification, von Neumann analysis, modified PDE.
- Convergence $\Rightarrow$ solve the correct problem, LR equivalence theorem.

5 Compressible flow

We considered the general compressible Navier–Stokes equation,

$$\frac{\partial \underline{U}}{\partial t} + \nabla \cdot \underline{\underline{F}} = \underline{Q} \ . \tag{5.1}$$

The *conservative* variables are ρ, ρu, ρv, ρw and E (*i.e.* density, momentum and energy)

$$\underline{U} = \begin{pmatrix} \rho \\ \rho \underline{u} \\ E \end{pmatrix} \qquad E = \rho(e + \frac{1}{2}\underline{u}^2) \ , \tag{5.2}$$

where E and e are the total energy and the internal energy, respectively, and $1/2\rho\underline{u}^2$ the kinetic energy. The *flux function* $\underline{\underline{F}}$ is given by

$$\underline{\underline{F}} = \begin{pmatrix} \rho \underline{u} \\ \rho \underline{u}\,\underline{u} + p\underline{\underline{I}} + \underline{\underline{\tau}} \\ (E+p)\underline{u} - \underline{\underline{\tau}} \cdot \underline{u} - k\nabla T \end{pmatrix} \ , \tag{5.3}$$

where $\underline{\underline{\tau}}$ is the viscous stress and the $-k\nabla T$ the heat dissipation and the thermal conductivity k. The (nonlinear) tensor (outer) product is defined as

$$\underline{u}\,\underline{u} = \begin{pmatrix} uu & uv & uw \\ vu & vv & vw \\ wu & wv & ww \end{pmatrix} \ . \tag{5.4}$$

The external forces are typically

$$\underline{Q} = \begin{pmatrix} 0 \\ \rho \underline{g} \\ Q \end{pmatrix} \ , \tag{5.5}$$

where $\underline{g}$ and Q are the gravity vector and a heat source, respectively.
This represent the most general description of a fluid flow (gas, liquid, etc.), within the continuous approximation. In order to close the system, a model is needed for the viscous stress: in case of a Newtonian fluid we have

$$\underline{\underline{\tau}} = \mu \left(\nabla \underline{u} + \nabla \underline{u}^T - \left(\frac{2}{3} \nabla \cdot \underline{u} \right) \underline{\underline{I}} \right) \tag{5.6}$$

as well as relations to connect E, p and $\underline{u}$, for instance the ideal gas model. In order to be able to simplify these equations, and only consider the most relevant terms, the two major distinctions are:

- viscous / inviscid flow $\Rightarrow \tau = 0$;
- compressible / incompressible flow $\Rightarrow$ constant ρ (along fluid trajectories $D\rho/Dt = 0$).

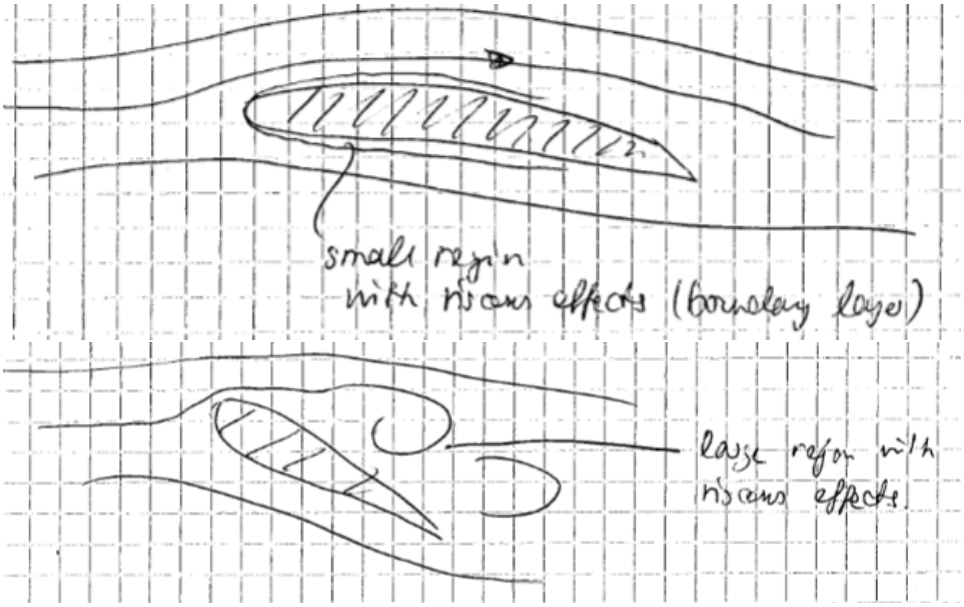


Figure 5.1: Wing profile (top) without and (bottom) with separation.

When is a flow compressible? A *fluid* (gas, liquid) is always compressible to some extent. However, in a specific *flow* situation, compressibility may be neglected.

- incompressible flow: conditions such that the they cause small pressure changes in the fluid;
- large pressure changes (waves)

Rule of thumb: Incompressible consideration is sufficient for gases when $u \leq 0.3c$, where c is the speed of sound, which is in general expressed in terms of the Mach number M:

$$M = \frac{u}{c} \leq 0.3 \tag{5.7}$$

When is a flow inviscid? When viscous effect are not important, *e.g.:* far away from walls, in absence of separation and at high Reynolds number $\Rightarrow$ outside the boundary layer region, see Fig. 5.1.

5.1 Euler equations

Assuming the flow inviscid and compressible, we obtain the Euler equations:

$$\frac{\partial \underline{U}}{\partial t} + \nabla \cdot \underline{F} = \underline{Q}\,, \tag{5.8}$$

where:

$$\underline{U} = \begin{pmatrix} \rho \\ \rho\underline{u} \\ E \end{pmatrix} \qquad \underline{F} = \begin{pmatrix} \rho\underline{u} \\ \rho\underline{u}\underline{u} + p\underline{\underline{I}} \\ (E+p)\underline{u} \end{pmatrix} \qquad \underline{Q} = 0 \qquad E = \rho\left(e + \frac{1}{2}\underline{u}^2\right) \tag{5.9}$$

These are 5 equations for 6 unknowns, ρ, $\underline{u}$, p and e. An additional equation is required from thermodynamics

$$e = e(T, p) \ . \tag{5.10}$$

For an ideal gas (like air) $e = e(T)$ and:

$$p = \rho R T \tag{5.11}$$

$$e = c_V T \tag{5.12}$$

$$c_V = \frac{R}{\gamma - 1} \qquad \gamma = \frac{c_P}{c_V} \simeq 1.4 \,(\text{for air}) \tag{5.13}$$

Here R is the specific gas constant, $R = \overline{R}/M$, where $\overline{R} = 8.314\text{J}/(\text{K} \cdot \text{mol})$ and M the molar mass in kg/mol, $c_v = (\partial e/\partial T)_\rho$ and $c_p = (\partial h/\partial T)_p$ (the enthalpy, $h = e + p/\rho$) are the amount of heat absorbed per unit mass of fluid per unit rise in temperature (specific heat), respectively, and γ is the *adiabatic index*. With these equations, one can build the required *equation of state*

$$p = \rho(\gamma - 1)e \qquad \gamma = \frac{c_P}{c_V} \simeq 1.4 \,(\text{for air}) \ . \tag{5.14}$$

Equations (5.9) and (5.14) form a complete system for compressible inviscid flow of an ideal gas (without considering chemical reactions).

5.2 Type classification

Considering the 1D case, in conservative form: $\underline{U}_t + \underline{F}_x = 0$.

$$\underline{U} = \begin{pmatrix} \rho \\ \rho u \\ (p+E)u \end{pmatrix} \qquad F(\underline{U}) = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ (E+p)u \end{pmatrix} \tag{5.15}$$

$$E = \rho(e + \frac{1}{2}u^2) \qquad p = (\gamma - 1)\rho \cdot e \tag{5.16}$$

As done earlier, we can rewrite it as $\underline{V}_t + \underline{\underline{A}}\,\underline{V}_x = 0$, which is the so-called *quasi-linear* form

$$\underline{V} = \begin{pmatrix} \rho \\ u \\ p \end{pmatrix} \qquad \underline{\underline{A}} = \begin{pmatrix} u & \rho & 0 \\ 0 & u & 1/\rho \\ 0 & \rho c^2 & u \end{pmatrix} \qquad \text{with } c^2 = \frac{\gamma p}{\rho} = \left.\frac{\partial p}{\partial \rho}\right|_{\text{ad}} , \tag{5.17}$$

where in the adiabatic limit $p = k \cdot \rho^{\gamma}$. The system has three eigenvalues

$$\lambda_1 = u,\ \lambda_2 = u + c,\ \lambda_3 = u - c\ . \tag{5.18}$$

Since λ_i are all real, the system is of hyperbolic type. Therefore, we can state that the Euler equations represent a non-linear, hyperbolic system of equations with three conservative variables density ρ, momentum ρu and energy E.

5.3 Non-linear conservation laws

Consider the problem in so-called *conservative* (or divergence) form:

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} f(u) = 0 \tag{5.19}$$

The *quasi-linear* (or convective) form is:

$$\frac{\partial u}{\partial t} + f' \frac{\partial u}{\partial x} = 0 \tag{5.20}$$

The characteristics are:

$$\frac{\mathrm{d}u}{\mathrm{d}t} = u_t + \frac{\mathrm{d}x}{\mathrm{d}t} u_x = 0 \qquad \text{with } \frac{\mathrm{d}x}{\mathrm{d}t} = f' = \lambda \tag{5.21}$$

The solution is thus constant along lines

$$\frac{\mathrm{d}x}{\mathrm{d}t} = f'\ . \tag{5.22}$$

Example 5.1 ***Advection equation*:**

$$f(u) = au,\ f' = a \quad \Rightarrow \quad \frac{\mathrm{d}x}{\mathrm{d}t} = \lambda = a\,, \tag{5.23}$$

which represent constant advection with velocity a. □

Example 5.2 ***Burgers equation*:**

$$f(u) = \frac{1}{2}u^2,\ f' = u \tag{5.24}$$

Since the characteristics can cross, discontinuity may develop (shock), despite smooth initial condition: *this is a feature of non-linear conservation laws.* This was already shown in Fig. 1.8 above. □

5.3.1 Conservation property of a conservation law

What is actually conserved when applying a conservation law? For that we consider a canonical form,

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} f(u) = 0 \ . \tag{5.25}$$

Integrate in $-\infty < x < \infty$:

$$\int_{-\infty}^{+\infty} (u_t + f_x)\,\mathrm{d}x = \frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{+\infty} u\,\mathrm{d}x + f(u)\Big|_{-\infty}^{+\infty} = 0 \quad \Rightarrow \tag{5.26}$$

If we assume $f(u) \to 0$ for $x \to \pm\infty$ (no flux at $\pm\infty$):

$$\Rightarrow \quad \frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{+\infty} u\,\mathrm{d}x = 0 \tag{5.27}$$

Therefore, we see that the integral of the quantity u is conserved in the full domain. If one wants to work with a smaller domain, by integrating in the finite interval $a \le x \le b$ we obtain the integral form:

$$\underbrace{\frac{\mathrm{d}}{\mathrm{d}t}\int_a^b u\,\mathrm{d}x}_{\text{total quantity}} = \underbrace{f(u(a,t))}_{\text{“flux” in at } a} - \underbrace{f(u(b,t))}_{\text{“flux” in at } b} \ . \tag{5.28}$$

This equation means that the change inside the considered domain is equal to what comes in minus what goes out. The numerical approximation should respect this property: **conservative formulation**. Use this form for discontinuous u, since no derivatives are necessary.

5.3.2 Riemann problem

In order to understand the behaviour of nonlinear conservation laws, we consider two canonical situations, namely a single step, either from high to low, or from low to high. This simplified case has become know as a *Riemann problem*, and is used as a test problem for numerical algorithms. Let us consider the following Riemann problem with the Burgers flux

$$u_t + f(x)_x = 0 \qquad f(u) = \frac{1}{2}u^2 \ , \tag{5.29}$$

$$u_0(x) = \begin{cases} u_L & \text{if } x \le 0 \\ u_R & \text{if } x > 0 \end{cases} \tag{5.30}$$

The initial data has only two constant values. The characteristics are the lines with slope:

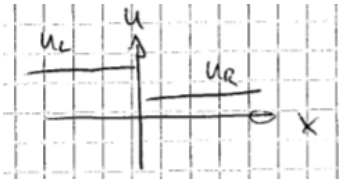


Figure 5.2: Initial conditions of the Riemann problem.

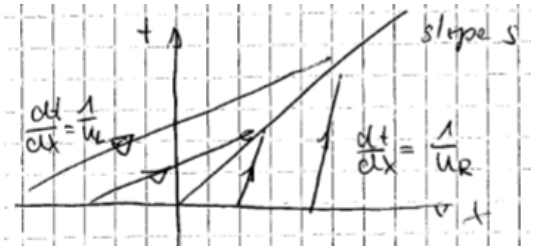


Figure 5.3: Shock (intersection of the characteristics).

$$\frac{\mathrm{d}x}{\mathrm{d}t} = f'(u) = u \tag{5.31}$$

The shock speed (intersection of the characteristics) is given by the Rankine–Hugoniot condition

$$s = \left.\frac{\mathrm{d}x}{\mathrm{d}t}\right|_s = \frac{f(u_L) - f(u_R)}{u_L - u_R} = \frac{1}{2}(u_R + u_L) \ , \tag{5.32}$$

where the last equation only holds for the specific case of the Burgers equation. In this case, the general solution is to the given initial condition is

$$u(x,t) = \begin{cases} u_L & \text{if } x - st < 0 \\ u_R & \text{if } x - st \geq 0 \end{cases} \ . \tag{5.33}$$

Note that s is **not** the speed of the characteristics (as in the linear case, speed a).

Since we deal with physical problems, even discontinuous solutions should satisfy basic physical (thermodynamics) properties. **Entropy condition:** Entropy S is a measure of the "disorder" of a system. It indicates how much of the inner energy in a system is available to do useful work (*e.g.:* increase pressure, decrease density, etc.).

- smooth flows: entropy is constant along fluid path (*isentropic* flows).
- shocks: entropy should increase: $f'(u_L) > s > f'(u_R)$ over a shock. This condition essentially says that characteristics need to go into a shock, not originate in the shock.

For the case of the Burgers flux, the entropy condition translates to

$$u_L > \frac{1}{2}(u_R + u_L) > u_R \ , \tag{5.34}$$

i.e. the speed on the left needs to be larger than the speed on the right for a shock to appear (since $u_L > u_R$). In the considered case the shock is indeed increasing the entropy and is thus a physical solution.

Consider now the opposite conditions $u_L < u_R$, illustrated in Fig. 5.4. Here two options are either an "expansion shock", or a smooth expansion

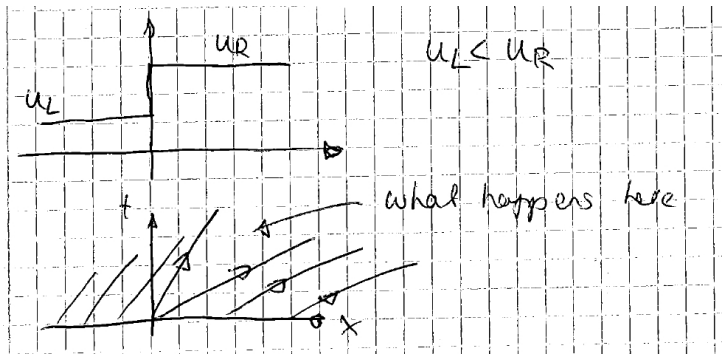


Figure 5.4: Riemann problem with $u_L < u_R$.

wave. The shock solution would not fulfill the entropy condition ($u_L > \frac{1}{2}(u_R + u_L) > u_R$ which is inconsistent with $u_L < u_R$) and is thus not a physical solution. Thus the smooth *expansion fan* or *rarefaction wave* is appearing, *i.e.* a smooth (linear) transition from u_L to u_R. This is a solution in the classical sense and we do not need the entropy condition.

The two physical solutions to the Riemann problem with either $u_L > u_R$ and $u_L < u_R$ are summarised in Fig. 5.5. We can thus easily sketch the solution in both cases. Doing this consideration in every point can potentially be used to construct the solution of a conservation law even in larger domains with more complex initial conditions.

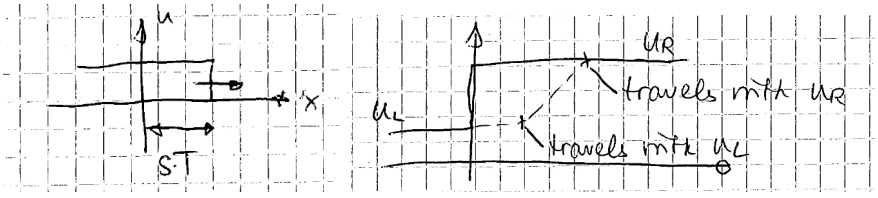


Figure 5.5: Solution to the Riemann problem for (left) $u_L > u_R$ and (right) $u_L < u_R$.

5.3.3 Connection to physical problem

A hyperbolic problem (at least as a math model for physics) is often an approximation to a problem with small viscosity.
For the Burger equation:

$$u_t + \left(\frac{1}{2}u^2\right)_x = 0 \quad \Rightarrow \quad u_t + \left(\frac{1}{2}u^2\right)_x = \varepsilon u_{xx} \tag{5.35}$$

ε is small and therefore neglected. A physical shock is actually not discontinuous, but has very steep gradient.

5.3.4 Derivation of the Rankine–Hugoniot condition

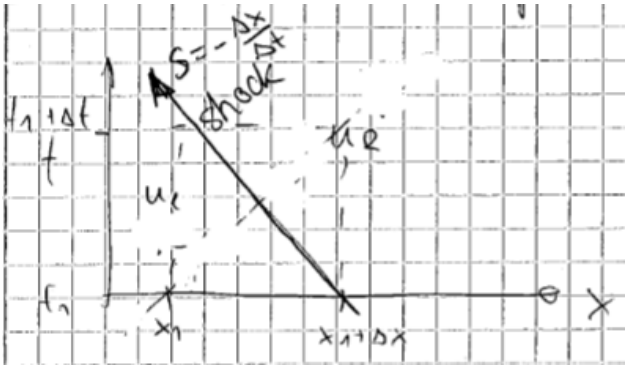
In order to derive the speed of shocks, the so-called *Rankine–Hugoniot condition*, we start with a generic conservation law,

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} f(u) = 0 \ . \tag{5.36}$$

In the integral form:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{x_1}^{x_2} u \mathrm{d}x = f(u)\Big|_{x_1} - f(u)\Big|_{x_2} \tag{5.37}$$

Consider small a x/t-plane:



$$\begin{aligned} \int_{x_1}^{x_1+\Delta x} u(x, t_1 + \Delta t)\, \mathrm{d}x - \int_{x_1}^{x_1+\Delta x} u(x, t_1) \mathrm{d}x = \\ \int_{t_1}^{t_1+\Delta t} f(u(x_1)) \mathrm{d}t - \int_{x_1}^{t_1+\Delta t} f(u(x_1 + \Delta x) \mathrm{d}t \end{aligned} \tag{5.38}$$

with u being constant:

$$\Delta x \cdot u_R - \Delta x \cdot u_l = \Delta t f(u_L) - \Delta t f(u_R) + \mathcal{O}(\Delta t^2) \tag{5.39}$$

assuming $s = -\frac{\Delta x}{\Delta t}$:

$$-\frac{\Delta x}{\Delta t}(u_l - u_r) = f(u_L) - f(u_R) + \mathcal{O}(\Delta t) \tag{5.40}$$

In the limit $\Delta t \to 0$

$$s = \frac{f(u_R) - f(u_L)}{u_R - u_L} \ , \tag{5.41}$$

which is the Rankine–Hugoniot condition. As stated above, for the Burgers flux $f(u) = u^2/2$, one gets $s = (u_R + u_L)/2$.

6 Numerical methods for hyperbolic problems

6.1 A first example

Example 6.1 ***Burgers equation in convective form*:** Solve the Burgers equation in non-conservative (convective) form:

$$u_t + u \cdot u_x = 0 \qquad u_0(x) = \begin{cases} 1 & x < 0 \\ 0 & x \geq 0 \end{cases} \tag{6.1}$$

The exact solution is a shock moving to the right with speed s (Rankine-Hugoniot condition),

$$s = \frac{f(u_L) - f(u_R)}{u_L - u_R} = \frac{1}{2} \, . \tag{6.2}$$

Let consider a simple upwind scheme:

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x} u_j^n (u_j^n - u_{j-1}^n) \tag{6.3}$$

with initial condition:

$$u_j^0(x) = \begin{cases} 1 & x < 0 \\ 0 & x \geq 0 \end{cases} \tag{6.4}$$

Compute:

$$u_j^1 = u_j^0 - \frac{\Delta t}{\Delta x} \cdot u_j^0 (u_j^0 - u_{j-1}^0) \tag{6.5}$$

$u_j^0 - u_{j-1}^0 = 0 \, , \forall j$ except: $j = 0$, but at $j = 0$ is u_0^0, thus: $u_j^1 = u_j^0 \, , \forall j$. This continues for subsequent time steps, therefore the numerical solution converges to the solution:

$$u(x,t) = u_0(x) \tag{6.6}$$

which is obviously incorrect, and would not even converge for a finer grid spacing in space and time. The shock speed is estimated to $s = 0$ as opposed to the correct result $s = 1/2$. Considering the integrated value of u shows that for negative x there is an influx $f = 1$, and for positive x a flux of $f = 0$. This shows that the numerical scheme does not conserve u. It is thus better to approximate the conservative formulation $u_t + f(u)_x = 0$ instead, which would, even in its discretised form, conserve u. □

6.2 CFL condition

Let us go a step backward and consider the advection equation,

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0 \, . \tag{6.7}$$

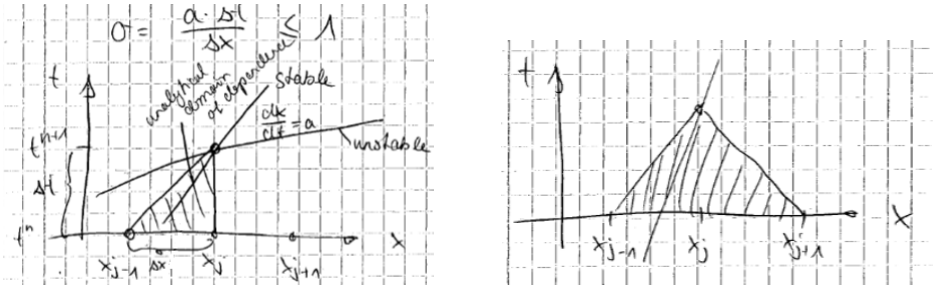


Figure 6.1: Domain of dependence for (left) upwind and (right) central difference schemes.

With the von Neumann analysis we found that the upwind/FTBS scheme is stable for

$$\sigma = \frac{a\Delta t}{\Delta x} \leq 1 \qquad (a > 0) \; . \tag{6.8}$$

The above criterion is called *CFL* (Courant–Friedrichs–Lewy, 1928) condition, and σ is a the Courant number.

Interpretation: a necessary condition for stability is that the domain of dependence of the FD scheme should include the domain of dependence of the PDE. The information should not travel more than one grid point. Note that the maximum σ is a function of the underlying PDE and the time-integration scheme.

Upwind schemes need to be always in the direction of the characteristics.

Example 6.2 ***CFL condition for central schemes*:** Consider a central difference schemes (FTCS):

$$u_j^{n+1} = u_j^n - \frac{a\Delta t}{2\Delta x}(u_{j+1} - u_{j-1}) \tag{6.9}$$

Let us perform the von Neumann analysis, substituting $u_j^n = \hat{u}_k^n \, e^{ikx_j}$:

$$\hat{u}_k^{n+1} = \hat{u}_k^n \left(1 - \underbrace{\frac{a\Delta t}{2\Delta x}\left(e^{ik\Delta x} - e^{-ik\Delta x}\right)}_{-i\sigma \sin(k\Delta x)} \right) \quad \Rightarrow \quad \hat{u}(k) = 1 - i\sigma \sin(k\Delta x) \tag{6.10}$$

$$\Rightarrow \quad |\hat{u}(k)|^2 = 1 + \sigma \sin^2(k\Delta x) > 1 \, , \tag{6.11}$$

where $\sigma = \frac{a\Delta t}{\Delta x}$, therefore this numerical scheme is unconditionally unstable! Although the CFL condition is fulfilled, the scheme is unstable: the CFL condition is only necessary, not sufficient! □

Example 6.3 ***Burgers equation*:** Let us now consider the Burgers equation in conservative form:

$$u_t + f(u)_x = 0 \qquad u(x,0) = \begin{cases} -1 & x \leq 0 \\ 1 & x > 0 \end{cases} \qquad u_L < u_R\,, \tag{6.12}$$

where $f(u) = u^2/2$ and $f'(u) = u$. As we know, the local speed of the characteristics is $a = f'(u)$. Considering the direction of propagation for the solution, we need to use a different discretization scheme, dependent on the local speed a (thus dependent on the local solution), *i.e.* upwind based on the fluxes between x_j and x_{j+1}, or between x_j and x_{j-1}. We can thus formally write

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x}\left(h_{j+1/2}^n - h_{j-1/2}^n\right)\,, \tag{6.13}$$

where $h_{j+1/2}^n$ and $h_{j-1/2}^n$ are approximations to the two fluxes on the left and on the right of grid point j; denoted with the position $j-1/2$ and $j+1/2$. Such a generic form of the discretised conservation law (6.13) is called *conservative* as it mimics the conservation properties of the underlying integral form of the conservation law. We can thus construct the appropriate differences depending on the local speed $f'(u_j)$ as follows,

$$\begin{aligned} h_{j+1/2} &= \begin{cases} f(u_{j+1}) \text{ for: } f'(u_j) < 0 \\ f(u_j) \text{ for: } f'(u_j) \geq 0 \end{cases} \\ h_{j-1/2} &= \begin{cases} f(u_j) \text{ for: } f'(u_{j-1}) < 0 \\ f(u_{j-1}) \text{ for: } f'(u_{j-1}) \geq 0 \end{cases} \end{aligned} \quad . \tag{6.14}$$

In the specific case of the example:

- $x_j < 0$:

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x}\left(f(u_{j+1}^n) - f(u_j^n)\right) \tag{6.15}$$

- $x_j > 0$:

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x}\left(f(u_j^n) - f(u_{j-1}^n)\right) \tag{6.16}$$

The scheme "decides" on its own which direction of the difference to take. However, this would not work for shocks, for which it is better to take central differences (*i.e.:* use x_{j+1} and x_{j-1}). An example is the (conditionally stable) Lax–Friedrichs scheme:

$$u_j^{n+1} = \underbrace{\frac{1}{2}\left(u_{j-1}^n + u_{j+1}^n\right)}_{\text{central space}} - \frac{\Delta t}{2\Delta x}\underbrace{\left(f(u_{j+1}^n) - f(u_{j-1^n})\right)}_{\text{central space}}\,. \tag{6.17}$$

□

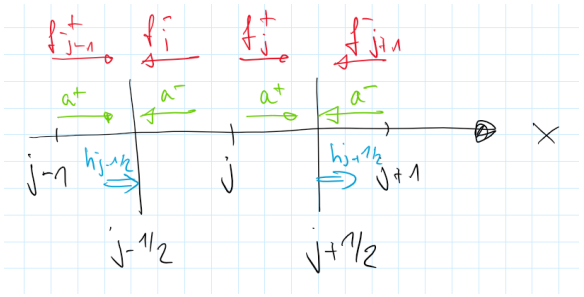


Figure 6.2: Idea of conservative form and flux splitting for grid point j.

A more general way of expressing the same idea can be obtained with the so-called *flux splitting*, as illustrated in Fig. 6.2. For the case of advection of a scalar ϕ with velocity a, we can define two speeds using the (local) speed a_j,

$$\begin{aligned} a_j^+ &= \max(a_j, 0) = \frac{1}{2}(a_j + |a_j|) \\ a_j^- &= \min(a_j, 0) = \frac{1}{2}(a_j - |a_j|) \end{aligned} , \tag{6.18}$$

where for positive a only $a^+ = a$ and $a^- = 0$, and associated fluxed

$$f_j^+ = a_j^+ u_j \,, \quad f_j^- = a_j^- u_j \,. \tag{6.19}$$

The two fluxes h for the conservative form (6.13) then become

$$h_{j-1/2} = f_{j-1}^+ + f_j^- , \tag{6.20}$$

$$h_{j+1/2} = f_j^+ + f_{j+1}^- \,. \tag{6.21}$$

6.3 Method of the modified differential equation

It is an alternative and more intuitive way to determine stability and behaviour of a numerical scheme. Consider the truncation error:

$$T(x_j, t^n) = P[v]_{x_j,t^n} - P_N[v_N]_{x_j,t^n} \tag{6.22}$$

Example 6.4 ***First-order scheme*:** Let consider the FTBS and for the advection equations:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = -a\frac{u_j^n - u_{j-1}^n}{\Delta x} \tag{6.23}$$

$$T(x_j, t^n) = \frac{1}{2}a\Delta x(1-\sigma)u_{xx} + \sigma(\Delta x^2, \, \Delta t^2) \tag{6.24}$$

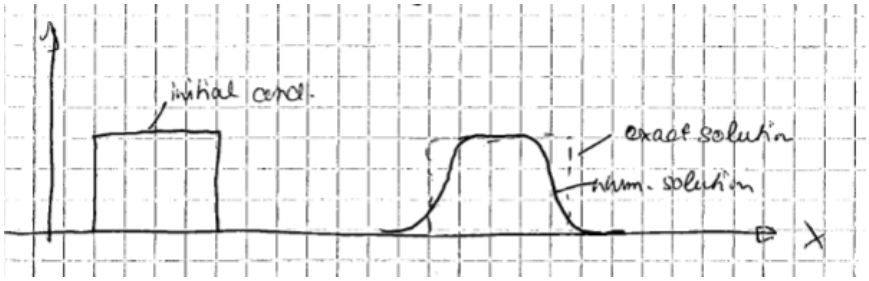


Figure 6.3: Effect of a diffusive term on a top-hat initial conditions.

If we retain this term, we see that we actually solve for:

$$u_t + a u_x = \underbrace{\frac{1}{2} a \Delta x (1-\sigma)}_{\nu_{\text{num}}} u_{xx} + \sigma(\Delta x^2, \Delta t^2)\,, \tag{6.25}$$

which is an advection/diffusion equation, whereas the equation was:

$$u_t + a u_x = 0 \tag{6.26}$$

The additional term resemble a viscosity, producing smoothing for $\nu_{\text{num}} > 0$:

$$\nu_{\text{num}} = \frac{1}{2} a \Delta x (1-\sigma) \quad \geq 0 \qquad (\text{for } a > 0)\,, \tag{6.27}$$

$$\Rightarrow \quad \sigma \leq 1 \tag{6.28}$$

What does this smoothing mean (see Fig. 6.3)?

- the smaller σ, the more dissipation;
- if $\sigma = 1 : \nu_{\text{num}} = 0$, exact solution;
- if $\sigma > 1 : \nu_{\text{num}} < 0$, inverse heat equation (blow-up!)

□

Example 6.5 ***Second-order scheme*:** In the following example, we construct a 2^{nd}-order scheme. Start with FTCS:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = -\frac{a}{2\Delta x}\left(u_{j+1}^n - u_{j-1}^n\right) \tag{6.29}$$

The modified PDE is:

$$u_t + a u_x = -\frac{1}{2} a^2 \Delta t u_{xx}\,, \tag{6.30}$$

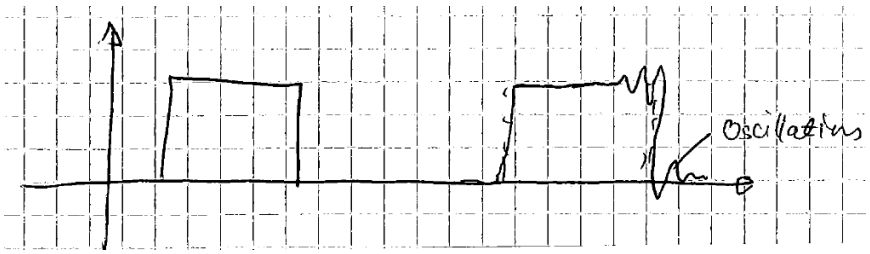


Figure 6.4: Effect of a dispersive term on a top-hat initial conditions.

unconditionally unstable due to negative diffusion. However, if we add a term this leading error term:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{a}{2\Delta x}\left(u_{j+1}^n - u_{j-1}^n\right) + \frac{1}{2}a^2\Delta t\frac{\Delta x^2}{u_{j-1}^n - 2u_j^n + u_{j+1}^n} \tag{6.31}$$

we get the Lax–Wendroff scheme (2^{nd} order in time and space). In this case, the modified PDE is:

$$u_t + au_x = \frac{1}{6}a\Delta x^2(\sigma^2 - 1)u_{xxx} + \dots\,, \tag{6.32}$$

where $\sigma = a\frac{\Delta t}{\Delta x}$, which is stable for $|\sigma| \leq 1$. Since the leading term in the modified PDE is $\propto u_{xxx}$, the numerical solution will have a *dispersive behaviour*. □

"Dispersion" means that waves with different frequency have different propagation speed. As a discontinuity contains a broad spectrum, the time advancement leads to spurious oscillations when the numerical error has a dispersive behaviour. This is schematically illustrated in Fig. 6.4.

6.4 Non-linear stability

We have described earlier the von Neumann analysis: since it employed the Fourier transform and superposition, strictly it can be applied only for the linear problems. Let consider a non-linear problem:

$$u_t + f(u)_x = 0 \tag{6.33}$$

We can define the *quasi-linear form* as:

$$u_t + \underbrace{f'(u)}_{\text{non-constant}} \cdot u_x = 0 \tag{6.34}$$

To perform a non-linear stability analysis, we can linearise the problem, *i.e.* assume

$$u = U + u'\,, \tag{6.35}$$

where U is a constant and u' a small perturbation. Substitute equation (6.35) into equation (6.33) yields

$$U_t + u'_t + f(U + u')_x = 0 \ . \tag{6.36}$$

Since U is constant, $U_t = 0$ and, since we assume $u' \ll U$, it is possible to use the Taylor expansion to express the term with the x derivative:

$$f(U + u')_x = f(U)_x + f'(U)u'_x + \mathcal{O}(u'^2) \tag{6.37}$$

$f(U)_x = 0$, therefore, at first order in u':

$$u'_t + \underbrace{f'(U)}_{\text{constant = a}} u'_x = 0 \tag{6.38}$$

The von Neumann analysis can be performed on the linearised problem (6.38).

Example 6.6 ***Upwind scheme*****:** For the (linear) advection equation (speed a) discretised with a first order upwind scheme (FTBS), we found the following stability limit

$$\left| \frac{a\Delta t}{\Delta x} \right| \leq 1 \ . \tag{6.39}$$

Using the above linearisation, one gets

$$\left| f'(U) \frac{\Delta t}{\Delta x} \right| \leq 1 \ . \tag{6.40}$$

In practise, assume that u' is small:

$$f'(U) \approx f'(U + u') = f'(u) \tag{6.41}$$

then, *e.g.* for the current upwind scheme, use:

$$\left| \frac{f'(u)\Delta t}{\Delta x} \right| \leq 1 \tag{6.42}$$

as stability bound. Note that $f'(u)$ varies in time and space, so the actual condition is for each time step,

$$\Delta t \leq \min_j \frac{\Delta x_j}{|f'(u_j)|} = \frac{\Delta x}{\max_j |f'(u_j)|} \ , \tag{6.43}$$

with the last equality for cases with constant grid spacing Δx. □

Example 6.7 ***Burgers equation*****:**

$$f(u) = \frac{1}{2}u^2 \qquad f'(u) = u \tag{6.44}$$

with the above upwind scheme of first order and constant Δx

$$\Delta t \leq \frac{\Delta x}{|\max(u)|} \ . \tag{6.45}$$

□

Example 6.8 ***Second-order scheme*****:** We consider now the MacCormack scheme which is simpler to implement than Lax-Wendroff (and very popular during 70s–80s). It is a two-steps scheme, also so-called *Predictor-Corrector* scheme:

$$\begin{cases} u_j^* = u_j^n - \lambda \left(f(u_{j+1}^n) - f(u_j^n) \right) & \text{forward predictor} \\ u_j^{n+1} = \frac{1}{2}(u_j^n + u_j^*) - \frac{1}{2}\lambda \left(f(u_j^*) - f(u_{j-1}^*) \right) & \text{backward correction} \end{cases} \tag{6.46}$$

Here, $\lambda = \Delta t/\Delta x$. For the linear advection equation ($u_t + a u_x = 0$), the MacCormack scheme is identical to the Lax–Wendroff scheme, *i.e.*,

$$\sigma = \left| a \frac{\Delta t}{\Delta x} \right| \leq 1 \ . \tag{6.47}$$

Therefore, the non-linear stability is simply

$$\Delta t = \sigma \frac{\Delta x}{\max |f'(u)|} \ , \quad \text{with: } \sigma < 1 \ . \tag{6.48}$$

□

6.5 Example: Burgers equation

In this section, we present the results of time-integrating the Burgers equation in a domain $x = 0 \ldots 10$ with the piecewise constant initial conditions as in Fig. 6.5. The following conservative numerical schemes are used:

- Upwind scheme with automatic detection of upwind direction (flux splitting)
- Lax–Friedrichs scheme
- Lax–Wendroff scheme
- Flux limiting scheme with Van Leer limiter.

A snapshot of the solutions at $t = 5$ is shown in Fig. 6.6. It is quite obvious that the Lax–Friedrichs scheme is very diffusive, and all the shocks are completely removed. The (second-order) Lax-Wendroff scheme shows significant wiggles (oscillations) just ahead of discontinuities. However, the shock speed is predicted correctly. The first-order upwind scheme does not show any wiggles.

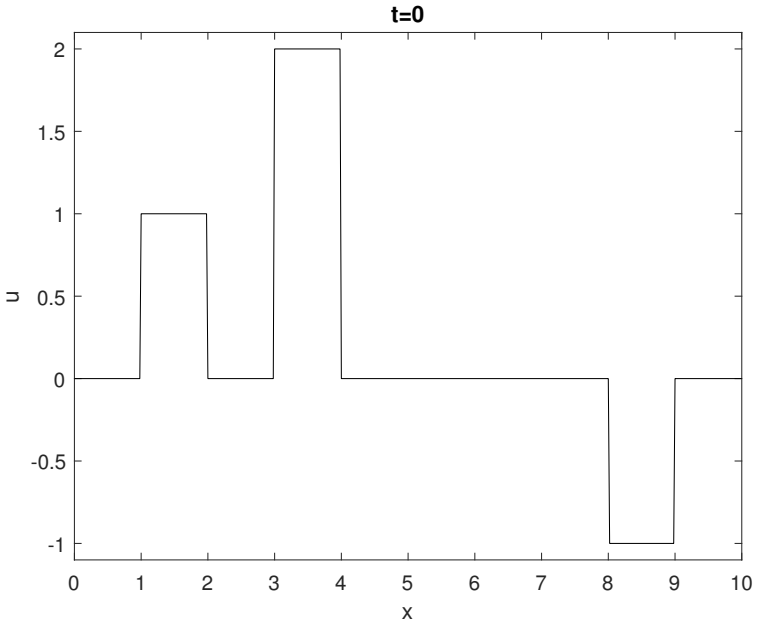


Figure 6.5: Initial condition at $t = 0$ for the Burgers equation.

The flux-limited scheme using the van Leer limiter switches automatically between the Lax–Wendroff and the upwind scheme depending on the local smoothness of the solution. As such this scheme attempts to combine the advantages of both the low and higher-order scheme. Therefore, it provides the most accurate prediction to the solution over the whole time evolution (see Fig. 6.7) with minimal dissipation, but yet without spurious oscillations. In particular, the prediction of the various shock speeds is most accurate.

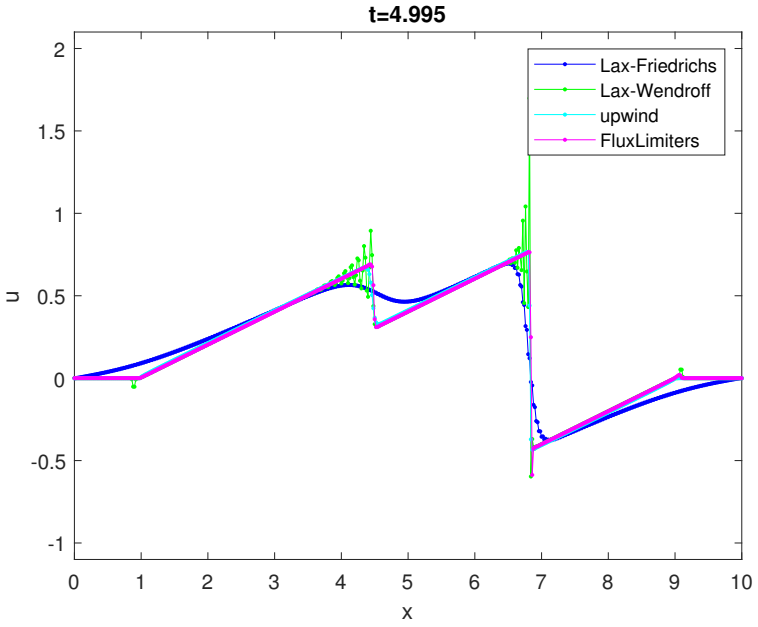


Figure 6.6: Snapshot at $t = 5$ for the Burgers equation, started from initial conditions as in Fig. 6.5.

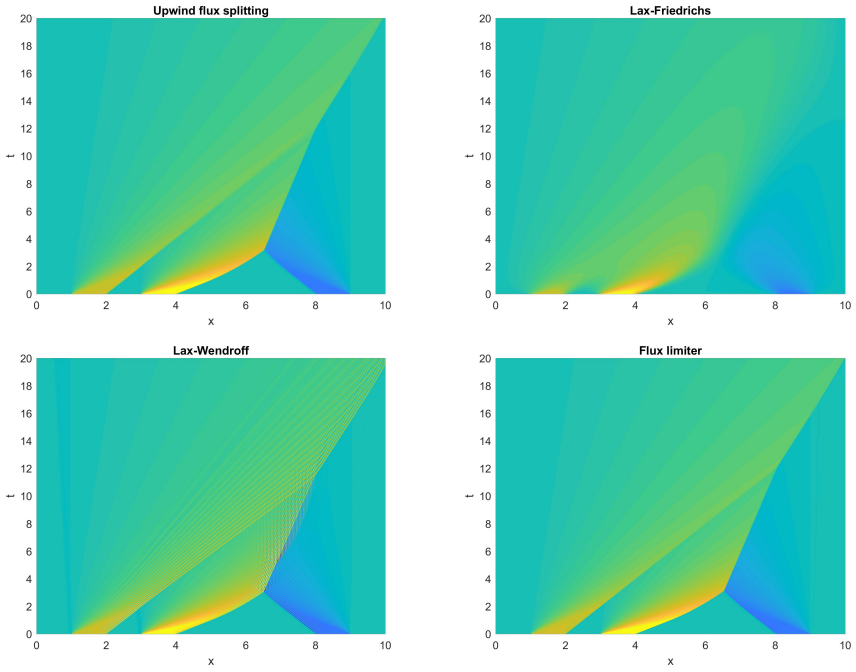


Figure 6.7: Space–time diagram for the Burgers solution from the initial condition shown in Fig. 6.5; colours from -1 (blue) till 2 (yellow).

7 Dispersive and dissipative errors

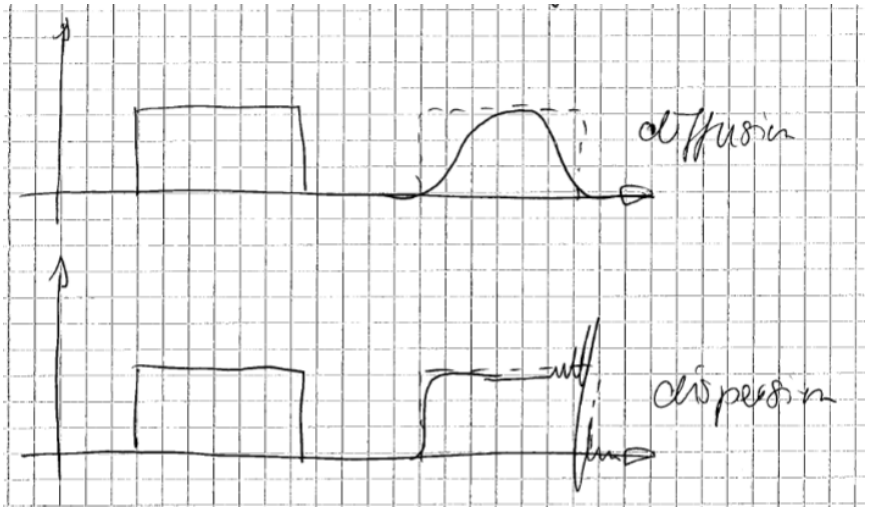


Figure 7.1: Dispersive and dissipative square wave.

As discussed before, the advection of a top-hat signal is shown in Fig. 7.1. To further understand these phenomena, let us consider a single wave

$$u(x,t) = \hat{u}\, e^{i(kx-\omega t)} \ . \tag{7.1}$$

The wave length L and the period T are defined:

$$L = \frac{2\pi}{k} \qquad T = \frac{2\pi}{\omega} \tag{7.2}$$

Phase velocity c_p and the group velocity c_g are:

$$c_p = \frac{L}{T} = \frac{\omega}{k} \qquad c_g = \frac{\partial \omega}{\partial k} \tag{7.3}$$

Example 7.1 ***Advection equation*:** For the advection equation $u_t + \lambda u_x = 0$:

$$\hat{u}e^{i(kx-\omega t)}(-i\omega) = -\lambda \hat{u} e^{i(kx-\omega t)}(ik) \quad \Rightarrow \quad \omega = \lambda k \tag{7.4}$$

This is called dispersion relation:

$$c_p = \lambda = c_g \tag{7.5}$$

waves move with speed $c_p = \lambda$, as expected from (7.1). □

Example 7.2 *Heat equation*: For heat equation $u_t = \nu u_{xx}$

$$\omega = -i\nu k^2 \quad \Rightarrow \quad u = \hat{u}e^{ikx}\, e^{-\nu k^2 t} \tag{7.6}$$

the wave propagation:

$$c_p = -i\nu k \qquad c_g = -2i\nu k \tag{7.7}$$

which leads to exponential decay for $\nu > 0$. □

Example 7.3 *Dispersive wave*: For a third-order equation,

$$u_t = \alpha u_{xxx} \quad \Rightarrow \quad \omega = \alpha k^3 \tag{7.8}$$

one gets the following dispersion relation:

$$c_p = \alpha k^2 \ , \quad c_g = 3\alpha k^2 = 3c_p \tag{7.9}$$

and thus

$$u = \hat{u}e^{i(kx-\alpha k^3 t)} = \hat{u}e^{ik(x-c_p t)} \ . \tag{7.10}$$

Here, c_p depends on k, such that waves with shorter wave lengths are travelling faster. □

The modified equation identifies the leading error term, responsible for the behaviour of the solution:

- upwind first order (FTBS): diffusive;
- Lax–Wendroff, second order: dispersive.

7.1 Artificial viscosity

Idea: control wiggles with controlled diffusion, *i.e.* artificial viscosity. In the proximity of shocks oscillations may appear when a second-order scheme is used. Reasons:

- dispersion of the wave propagation;
- resolution of the shock (also for steady shocks).

$$u_t + f(u)_x = \varepsilon u_{xx} \ , \quad \varepsilon \approx \Delta x \tag{7.11}$$

to replace $u_t + f(u)_x = 0$. The conservative form (for ε constant) is:

$$u_t + \underbrace{(f(u) - \varepsilon u_x)_x}_{\tilde{f}_x} = 0 \quad \Rightarrow \quad u_t + \tilde{f}(u)_x = 0 \tag{7.12}$$

where $\tilde{f}$ is a modified flux function. Because $\varepsilon \approx \Delta x$, the accuracy is reduced to first order. Therefore, it is added only around shocks (locally).

Example 7.4 ***Stability of viscous term*:** Consider the stability analysis of a second-order derivative, on the example of the diffusion equation:

$$u_t = \varepsilon u_{xx} \tag{7.13}$$

with central scheme for u_{xx}:

$$u_j^{n+1} = u_j^n + \frac{\alpha \Delta t}{\Delta x^2} \left(u_{j+1} - 2u_j + u_{j-1} \right) \tag{7.14}$$

The von Neumann analysis gives:

$$\frac{\varepsilon \Delta t}{\Delta x^2} \leq \frac{1}{2} \tag{7.15}$$

- stability very sensitive to refinement in Δx because of the square;
- usually implicit ($\rightarrow$ stable) schemes are used for viscous terms.

□

7.2 Shock tube

The so-called Sod shock tube is a simple but physical application of the one-dimensional Euler equation. It is named after Gary A. Sod, and was introduced in his JCP paper in 1978. Let us consider a tube, modelled as a one-dimensaionl domain, divided into two portions by a removable diaphragm. The fluid is initially at rest in both portions of the domain, *i.e.* $v_0 = v_1 = 0$, but the pressure is higher in the *driver* section than in the *driven* section: $p_0 > p_1$. A sketch is given in Fig. 7.2.

Once the membrane is removed, the system needs to reach a new position of equilibrium. The governing equations of the system are:

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix} \rho u \\ \rho u + p \\ (E + p)u \end{pmatrix} = 0 \tag{7.16}$$

The system has three characteristics

$$\lambda_1 = u \qquad \lambda_{2,3} = u \pm c \; . \tag{7.17}$$

Shock tubes are used as gas-dynamics instruments to measure different gas properties at high speed and high temperature. They are also used as a test and validation problem for numerical methods.

At $t = 0$ the fluid is at rest, see Fig. 7.3. At $t > 0$, once the membrane is removed (Fig. 7.4):

- between Regions **1** and **2** a rarefaction wave propagates to the left, decreasing pressure and density (smooth interface).

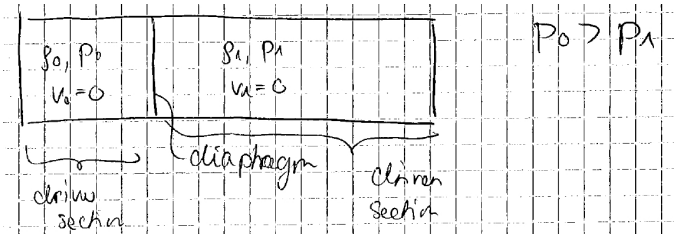


Figure 7.2: Initial conditions for the shock tube problem.

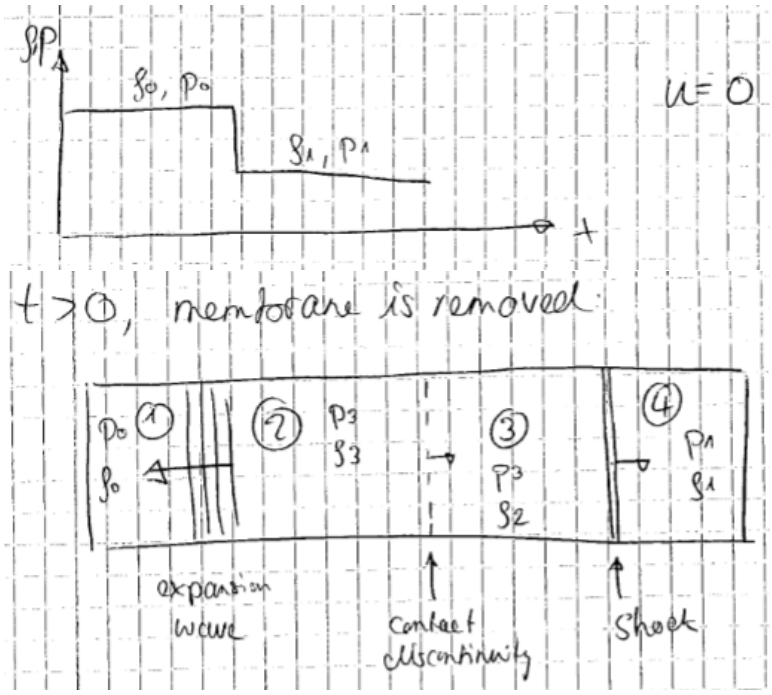


Figure 7.3: Shock tube (top) initial condition and (bottom) after removing the membrane.

- Regions **2** and **3** are separated by a contact discontinuity moving to the right. The pressure is constant, but not the density. This interface moves with the characteristic speed (not shock speed!)
- Between regions **3** and **4** a shock in both p and ρ forms, and propagates with the shock speed.

The simplification we may use is isentropic flow (see homeworks),

$$\frac{p}{\rho^\gamma} = K \qquad \gamma = 1.4 \; . \tag{7.18}$$

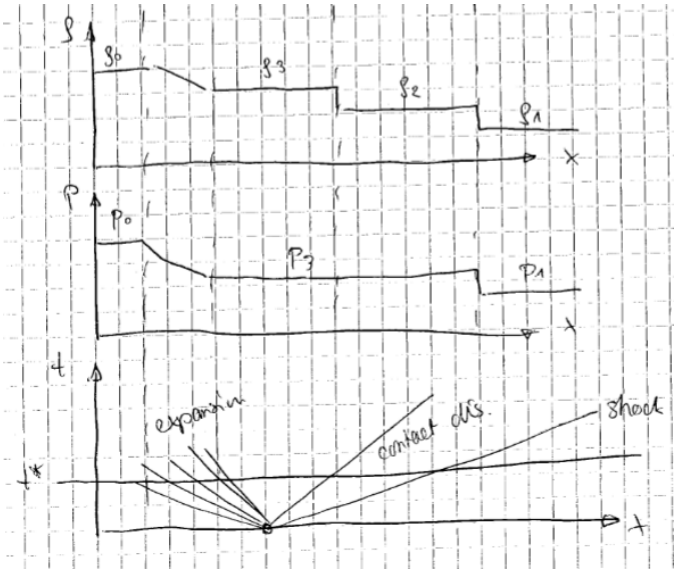


Figure 7.4: Evolution of the variables in the shock tube as a function of time and space.

Then we get

$$\begin{pmatrix} \rho \\ \rho u \end{pmatrix}_t + \begin{pmatrix} \rho u \\ \rho u^2 + p \end{pmatrix}_x = 0\,, \qquad \lambda_{1,2} = u \pm c \tag{7.19}$$

In the isentropic approximation, there will be no contact discontinuity (see also the eigenvalues) because the ratio p/ρ is fixed. We only get rarefaction wave and shock (not physical shocks $\rightarrow$ weak shock, otherwise entropy had to increase).

Initial and boundary conditions: At $t = 0$ the fluid is at rest, so $u = 0$, and $p/\rho^\gamma = K$. Also, p_0, T_0 and p_1 are given and:

$$\rho_0 = \frac{p_0}{RT_0} \qquad \frac{p_1}{\rho_1^\gamma} = \frac{p_0}{\gamma \rho_0^\gamma} = K \tag{7.20}$$

The boundary conditions need to be specified at each boundary, and their number needs to be at least equal to the number of in-going characteristics (see Section 7.3 below). The characteristics are the eigenvalues of F',

$$u = \begin{pmatrix} \rho \\ u \end{pmatrix} \qquad F' = \begin{pmatrix} u & \rho \\ c^2/\rho & u \end{pmatrix} \quad \Rightarrow \quad \lambda_{1/2} = u \pm c\,, \tag{7.21}$$

where c is the local speed,

$$c^2 = \frac{\gamma p}{\rho} = \gamma K \cdot \rho^{\gamma - 1}\,. \tag{7.22}$$

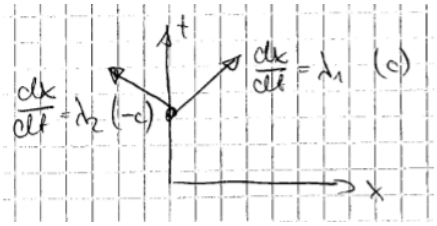


Figure 7.5: Characteristics in the shock tube for the isentropic approximation (*i.e.* only two variables/characteristics) at $x = 0$ (similarly for $x = L$).

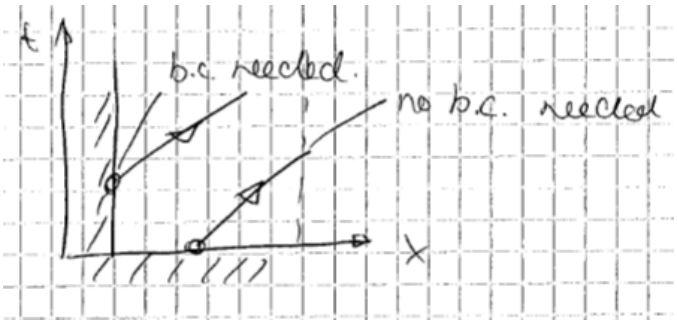


Figure 7.6: Boundary condition for a hyperbolic problem.

Look at the two walls located at $x = 0$ and $x = L$, where no-slip/no-penetration conditions apply (Fig. 7.5) ,

$$u = 0 \qquad \lambda_{1,2} = \pm c \; . \tag{7.23}$$

The unknowns are ρ and ρu. The *physical* boundary condition is $\rho u = 0$. There are however no physical condition from the boundary for ρ. The *numerical* boundary condition for ρ are thus obtained by extrapolation from inside the flow domain. The simplest way is

$$\rho(x = 0) = \rho_0 = \rho_1 \quad \text{(zeroth order extrapolation)}. \tag{7.24}$$

The formal derivation is based on Riemann invariants, as discussed further down in Section 8.

7.3 Boundary condition

For systems of conservation laws, there are conditions on the boundary conditions to be fulfilled in order for the problem to be well-posed. The number of boundary condition that have to be prescribed needs to be equal to the number of in-going characteristics, as illustrated in Fig. 7.6.

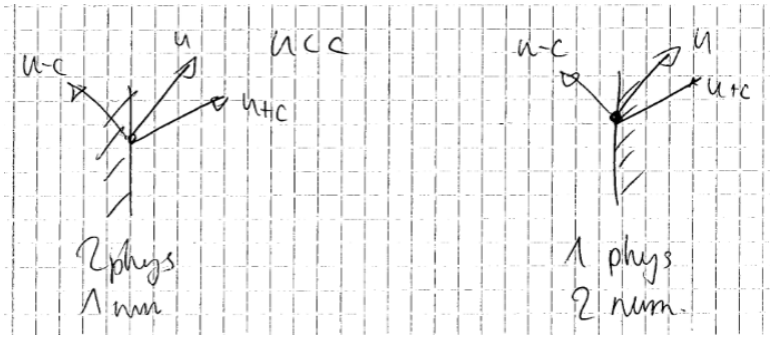


Figure 7.7: Boundary conditions for Euler in case of subsonic inflow and outflow.

Example 7.5 ***Hyperbolic problem*:**

$$\underline{u}_t + \underline{\underline{A}}(\underline{U})_x = 0 \qquad 0 \leq x \leq 1 \tag{7.25}$$

$\underline{\underline{A}} \in \mathbb{R}^{3\times 3}$ and we have 3 real eigenvalues λ_i. Assume λ_1, $\lambda_2 > 0$, $\lambda_3 < 0$. At $x = 0$, λ_1 and λ_2 are going into the domain (Fig. 7.7):

- two boundary conditions have to be given;
- only two values can be prescribed at $x = 0$.

The third variable will be given/determined by the solution inside the domain. At $x = 1$, the opposite situation occurs: only one boundary condition on the third variables can be prescribed. This mathematical constraint causes problems, when numerical boundary condition are needed. Numerical boundary conditions can be set by extrapolating from the inside of the domain (see also Riemann Invariants). □

Example 7.6 ***Euler with subsonic inflow/outflow*:** The previous example directly tells us what happens in the case of the Euler equations with the eigenvalues $\lambda_{1/2} = u \pm c$ and $\lambda_3 = u$. For subsonic inflow/outflow ($u < c$) we get the situation illustrated in Fig. 7.7, *i.e.* two characteristics travelling to the right, and one travelling to the left. In the supersonic case $u > c$, conversely, all characteristics are to the right, which means that three conditions at the inflow need to be given, but no physical condition at the outflow. □

8 Riemann Invariants

We will now in more detail study systems of conservation laws. Consider the general form

$$\underline{U}_t + \underline{\underline{A}} \cdot \underline{U}_x = 0 \qquad \underline{\underline{A}} \in \mathbb{R}^{m\times m}, \underline{U} \in \mathbb{R}^m \ . \tag{8.1}$$

The eigenvalues of $\underline{\underline{A}}$ are real, thus the system can be diagonalised via:

$$\underline{\underline{A}} = \underline{\underline{R}}\,\underline{\underline{\Lambda}}\,\underline{\underline{R}}^{-1} \tag{8.2}$$

where $\underline{\underline{R}}$ is the matrix containing the eigenvectors as columns, and $\underline{\underline{\Lambda}}$ is the diagonal matrix with eigenvalues on diagonal.

$$\begin{aligned} &\underline{\underline{A}}\,\underline{v}_i = \lambda_i \underline{v}_i \\ &\underline{\underline{A}}[\underline{v}_1\ \underline{v}_2 ...] = [\lambda_1\underline{v}_1\ \lambda_2\underline{v}_2 ...] = \underline{\underline{R}}\,\underline{\underline{\Lambda}} \\ &\underline{\underline{A}} \cdot \underline{\underline{R}} = \underline{\underline{R}} \cdot \underline{\underline{\Lambda}} \quad \Rightarrow \quad \underline{\underline{A}} = \underline{\underline{R}}\,\underline{\underline{\Lambda}}\,\underline{\underline{R}}^{-1} \end{aligned} \tag{8.3}$$

Multiplying (8.1) with $\underline{\underline{R}}^{-1}$:

$$\underbrace{\underline{\underline{R}}^{-1}\underline{U}_t}_{\underline{V}_t} + \underbrace{\underline{\underline{R}}^{-1}\underline{\underline{A}}\,\underline{\underline{R}}}_{\Lambda} \cdot \underbrace{\underline{\underline{R}}^{-1}\underline{U}_x}_{\underline{V}_x} = 0 \tag{8.4}$$

Define: characteristic variables:

$$\underline{V} = \underline{\underline{R}}^{-1} \cdot \underline{U} \quad \Rightarrow \quad \underline{V}_t + \underline{\underline{\Lambda}} \cdot \underline{V}_x = 0 \tag{8.5}$$

The equations are independent (decoupled) since Λ is diagonal. Same as:

$$\left(v^P\right)_t + \lambda^P \left(v^P\right)_x = 0 \tag{8.6}$$

which are m linear advection equation $p = 1 \ldots m$.
Solution: we know that v^P constant along $\frac{\mathrm{d}x}{\mathrm{d}t} = \lambda^P$. Therefore, v^P are called characteristic variables. Tracking these solutions is helpful when analysing the solution to conservation laws.
The initial condition is:

$$\underline{V}_0 = \underline{\underline{R}}^{-}1\underline{U}_0 \tag{8.7}$$

The solution is:

$$\underline{u}(x,t) = \underline{\underline{R}}\,\underline{V}(x,t) = \begin{pmatrix} \vdots & \vdots & \\ \underline{r}_1 & \underline{r}_2 & \ldots \\ \vdots & \vdots & \end{pmatrix} \cdot \begin{pmatrix} v_1 \\ v_2 \\ \vdots \end{pmatrix} \tag{8.8}$$

Solution:

$$\underline{u}(\underline{x},t) = \sum_{p=1}^{m} v^p(\underline{\lambda},t)\underline{r}_p = \sum_{p=1}^{m} v_0^p(\underline{x} - \lambda_p t)\underline{r}_p \tag{8.9}$$

This means that in each point in space the solution depends on a superposition of solutions that are given by v_P. Information coming from m characteristics given by the eigenvalues of $\underline{\underline{A}}$.

$$\underline{u} = \alpha v^1 + \beta v^2 + \gamma v^3 \tag{8.10}$$

where α, β and γ given by eigenvectors. Different components of the solution

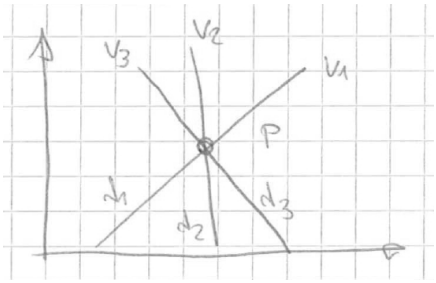


Figure 8.1: Schematic representation of the characteristics for a 3×3 system.

are constant along the characteristic lines, see also Fig. 8.1,

$$\begin{aligned} &v^1 \text{ along } \lambda_1 \\ &v^2 \text{ along } \lambda_2 \\ &v^3 \text{ along } \lambda_3 \end{aligned} . \tag{8.11}$$

Example 8.1 ***System of conservation laws*****:**

$$\frac{\partial}{\partial t}\underline{U} + \underline{\underline{A}}\frac{\partial \underline{U}}{\partial x} = 0 \tag{8.12}$$

where:

$$\underline{U} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \qquad \underline{\underline{A}} = \begin{pmatrix} a & b \\ b & a \end{pmatrix} \tag{8.13}$$

The domain is $0 \le x \le 1$.
The eigenvalues are $\lambda_{1,2} = a \pm b$ and the eigenvectors are $\underline{r}_{1,2} = \{1, \pm 1\}$:

$$\underline{\underline{R}} = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & -1/2 \end{pmatrix} \qquad \underline{\underline{R}}^{-1} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad \underline{\underline{\Lambda}} = \begin{pmatrix} a+b & 0 \\ 0 & a-b \end{pmatrix} \tag{8.14}$$

Characteristics variables:

$$\underline{V} = \underline{\underline{R}}^{-1} \cdot \underline{U} = \begin{pmatrix} u_1 + u_2 \\ u_1 - u_2 \end{pmatrix} = \begin{pmatrix} v^+ \\ v^- \end{pmatrix} \quad \Rightarrow \tag{8.15}$$

$$\Rightarrow \quad \begin{cases} v_t^+ + (a+b)v_x^+ = 0 \\ v_t^- + (a-b)v_x^- = 0 \end{cases} \tag{8.16}$$

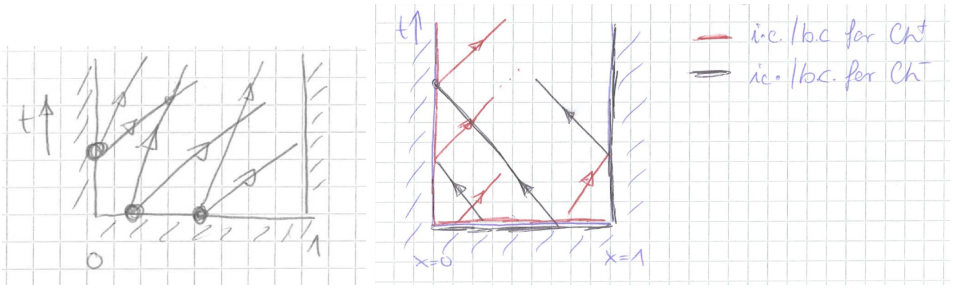


Figure 8.2: Boundary conditions for the hyperbolic problem given in the example. *Left:* $0 < b < a$, *right:* $0 < a < b$.

Along the characteristics Ch^+:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = a + b \; : \quad \frac{\mathrm{d}v^+}{\mathrm{d}t} = 0 \tag{8.17}$$

and along Ch^-:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = a - b \; : \quad \frac{\mathrm{d}v^-}{\mathrm{d}t} = 0 \tag{8.18}$$

The different possibilities for the boundary conditions are shown in Fig. 8.2. The following cases can be distinguished:

- $0 < b < a \Rightarrow$ both $\lambda_{1,2} > 0 \Rightarrow \mathrm{Ch}^+$ and Ch^- go to the right. Two conditions at $x = 0$, none at $x = 1$.
- $0 < b < a \Rightarrow \mathrm{Ch}^+$ towards right (λ_1) and Ch^- towards left (λ_2) one conditions at each boundary.

In the latter case, at $x = 0$:

$$v^+(0,t) = \alpha_0(t) v^-(0,t) + \beta_0(t) \tag{8.19}$$

at $x = 1$:

$$v^+(1,t) = \alpha_1(t) v^+(1,t) + \beta_1(t) \tag{8.20}$$

to be well-posed α_i, β_i are constant or functions of time. If we set, for example:

$$\begin{aligned} u_1(0,t) &= \frac{1}{2}\beta_0(t) \quad \text{at: } x = 0 \\ u_2(0,t) &= \frac{1}{2}\beta_1(t) \quad \text{at: } x = 1 \end{aligned} \tag{8.21}$$

For the characteristic variables:

$$\begin{aligned} &\underline{V_0} = \underline{\underline{R}}^{-1}\,\underline{U} \\ &v^+(x=0) = u_1(0,t) + u_2(0,t) = -v^-(x=0) + \beta_0(t) \\ &v^-(x=0) = u_1(1,t) + u_2(1,t) = v^+(x=1) - \beta_1(1) \end{aligned} \tag{8.22}$$

where $v^- = u_1 - u_2$ and $v^+ = u_1 + u_2$. The boundary conditions are a combination of given values and computed ones. □

Example 8.2 ***Euler equations*:** Consider the non-linear, isentropic, compressible 1D Euler equations:

$$\begin{pmatrix}\rho\\ u\end{pmatrix}_t + \begin{pmatrix}u & \rho\\ K\gamma\rho^{\gamma-2} & u\end{pmatrix}\cdot\begin{pmatrix}\rho & u\end{pmatrix}_x = 0 \quad \Rightarrow \tag{8.23}$$

with $K\gamma\rho^{\gamma-2} = c^2/\rho$, $c^2 = K\gamma\rho^{2\alpha}$ where $\alpha = (\gamma-1)/2$:

$$\Rightarrow \quad \underline{\underline{A}} = \begin{pmatrix}u & \rho\\ K\gamma\rho^{\gamma-2} & u\end{pmatrix} \tag{8.24}$$

determine type:

$$\det(\underline{\underline{A}} - \lambda I) = 0 \quad \Rightarrow \quad \lambda_{1,2} = u \pm c \tag{8.25}$$

Thus:

$$v_1 = \begin{pmatrix}\rho/2c\\ 1/2\end{pmatrix} \qquad v_2 = \begin{pmatrix}-\rho/2c\\ 1/2\end{pmatrix} \tag{8.26}$$

Diagonalise:

$$\Lambda = \begin{pmatrix}u+c & 0\\ 0 & u-c\end{pmatrix} = \underline{\underline{R}}^{-1}\,\underline{\underline{A}}\,\underline{\underline{R}} \tag{8.27}$$

with:

$$\underline{\underline{R}} = \begin{pmatrix}v_1 & v_2\end{pmatrix} \quad \text{and} \quad \underline{\underline{R}}^{-1} = \begin{pmatrix}c/\rho & 1\\ -c/\rho & 1\end{pmatrix} \tag{8.28}$$

Therefore, the characteristic form of (8.23) is:

$$\frac{\partial Z}{\partial t} + \Lambda\frac{\partial Z}{\partial x} = 0 \tag{8.29}$$

In principle this is a decoupled system, however due to non-linearity there is coupling through Λ. The new state vector Z is:

$$\omega_t + A\omega_x = 0\,, \quad \omega = \begin{pmatrix}\rho\\ u\end{pmatrix} \tag{8.30}$$

$$R\Lambda R^{-1} = A \quad \Rightarrow \quad \omega_t + R\Lambda R^{-1}\omega_x = 0 \tag{8.31}$$

$$\underbrace{R^{-1}\omega_t}_{Z_t} + \Lambda\,\underbrace{T^{-1}\omega_x}_{Z_x} = 0 \tag{8.32}$$

$$[Z_t]_i = \frac{\partial Z_i}{\partial\omega_j}[\omega_t]_j \quad \Rightarrow \quad \frac{\partial Z_i}{\partial\omega_j} = \left[R^{-1}\right]_{ij} \tag{8.33}$$

$$\begin{cases}\dfrac{\partial Z_1}{\partial\rho} = \dfrac{c}{\rho}\,, & \dfrac{\partial Z_2}{\partial\rho} = -\dfrac{c}{\rho}\\[2ex] \dfrac{\partial Z_1}{\partial u} = 1\,, & \dfrac{\partial Z_2}{\partial u} = 1\end{cases} \quad \Rightarrow \quad Z = u \pm \frac{c}{\alpha} \tag{8.34}$$

The two solutions Z are the Riemann invariants for the given problem. We know that along the characteristics $u \pm c$ the quantities $u \pm c/\alpha$ are constant:

$$\begin{pmatrix} u + c/\alpha \\ u - c/\alpha \end{pmatrix}_t + \begin{pmatrix} u + c & 0 \\ 0 & u - c \end{pmatrix} \begin{pmatrix} u + c/\alpha \\ u - c/\alpha \end{pmatrix}_x = 0 \tag{8.35}$$

The relevance is for specifying so-called characteristic boundary conditions. For instance, in the shock tube on the right boundary, there are 2 characteristics $u \pm c$ and one physical condition is imposed ($u = 0$). The numerical condition needs to be extrapolated from the inside:

$$Z_1 = u + \frac{c}{\alpha} = u + (\sqrt{K\gamma}/\alpha)\rho^\alpha \tag{8.36}$$

is constant along:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = u + c \tag{8.37}$$

At the wall $u = 0$, thus:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = c = \sqrt{K\gamma}\rho^\alpha \quad \Rightarrow \quad Z_1 = \text{const} = \left(\sqrt{K\gamma}/\alpha\right)\rho^\alpha \tag{8.38}$$

A zeroth order condition is $\rho = \text{const}$, but higher order is of possible (and desirable for high resolution schemes). □

9 Analysis of time integration

9.1 Analysis in one dimension

Consider advection-diffusion equation:

$$\frac{\partial u}{\partial t} + \underbrace{a\frac{\partial u}{\partial x}}_{\text{advection}} = \underbrace{\frac{1}{Re}\frac{\partial^2 u}{\partial x^2}}_{\text{diffusion}} \quad \text{FTCS for all terms} \tag{9.1}$$

Let us consider the terms independently (central differences)

- advection: CFL condition (only necessary):

$$\sigma = \frac{a\Delta t}{\Delta x} \leq 1 \tag{9.2}$$

- diffusion:

$$\beta = \frac{1}{Re}\frac{\Delta t}{\Delta x^2} \leq \frac{1}{2} \tag{9.3}$$

Considering the two terms together leads to (see study questions):

$$\sigma^2 \leq 2\beta \leq 1 \quad \Rightarrow \quad \begin{cases} \beta \leq \frac{1}{2} & \Leftrightarrow \quad \Delta t \leq \frac{1}{2}\Delta x^2 \cdot Re \\ \frac{\sigma^2}{\beta} \leq 2 & \Leftrightarrow \quad \Delta t \leq \frac{2}{Re\, a^2} \quad \text{indep. of } \Delta x! \end{cases} \tag{9.4}$$

- for low Re: *viscous time-step limit*;
- for high Re: the convection is stabilised by viscosity (remember, for $Re \to \infty$ the scheme is unstable!)

9.2 Analysis in two dimensions

$$\frac{\partial u}{\partial t} + a_x\frac{\partial u}{\partial x} + a_y\frac{\partial u}{\partial y} = \frac{1}{Re}\Delta u \tag{9.5}$$

CFL condition (only necessary condition), assuming $\Delta x = \Delta y$:

$$\sigma_x + \sigma_y \leq 1 \quad \Rightarrow \quad \Delta t \leq \left(\frac{|a_x|}{\Delta x} + \frac{|a_y|}{\Delta y}\right)^{-1} = \frac{\Delta x}{|a_x| + |a_y|} \tag{9.6}$$

Diffusion:

$$\beta_x + \beta_y \leq \frac{1}{2} \quad \Rightarrow \quad \Delta t \leq \frac{1}{2}Re\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right)^{-1} = \frac{1}{4}Re\Delta x^2 \tag{9.7}$$

Combination:

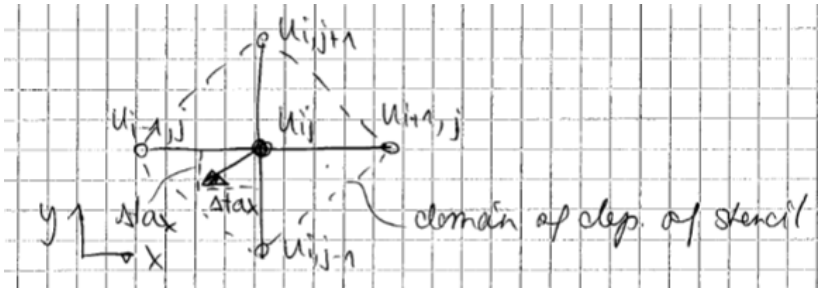


Figure 9.1: Sketch of the 2D stencil to determine the CFL condition.

- viscous limit:
$$\beta_x + \beta_y \leq \frac{1}{2} \tag{9.8}$$
- independent of Δx, Δy:
$$\frac{\sigma_x^2}{\beta_x} + \frac{\sigma_y^2}{\beta_y} \leq 2 \tag{9.9}$$

In practise: (test in the code!)

- viscous limit is necessary and sufficient (hard limit for low Re);
- CFL condition: only necessary, but easy to check;
- combined condition very strict (too strict) but necessary and sufficient.
- non-linearity: evaluate $a_x = |u|_{\max}$, $a_y = |v|_{\max}$

9.3 Derivation 2D CFL condition

According to the CFL condition, the domain of dependence of PDE needs to be fully contained within the domain of dependence of the numerical stencil. Let us consider the central approximation of the 2D advection equation, see Fig. 9.1:

$$\frac{\partial u}{\partial t} + a_x \frac{\partial u}{\partial x} + a_y = 0 \tag{9.10}$$

From the definition:

$$\Delta t \frac{|a_x|}{\Delta x} + \Delta t \frac{|a_y|}{\Delta y} \leq 1 \tag{9.11}$$

Similar for higher dimensions:

$$\Delta t \sum \frac{|a_i|}{\Delta x_i} \leq 1 \tag{9.12}$$

9.4 Stability of the diffusion equation in 2D

Recall the one-dimensional analysis for the diffusion equation,

$$\text{1D:} \qquad \frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2} \qquad \text{FTCS} \tag{9.13}$$

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{\nu}{\Delta x^2} \left(u_{j+1}^n - 2u_j^n + u_{j-1}^n \right) \ . \tag{9.14}$$

von Neumann analysis: $u_j^n = \hat{u}_k^n e^{ik\alpha x_j}$.

$$\hat{u}_k^{n+1} = \hat{u}_k^n + \frac{\nu \Delta t}{\Delta x^2} \underbrace{\left(e^{ik\alpha\Delta x} + e^{-ik\alpha\Delta x} \right)}_{2\cos\phi_k - 2,\ \phi_k = k\alpha\Delta x} \hat{u}_k^n \tag{9.15}$$

$$|\hat{G}_k| \leq 1 \quad \Rightarrow \quad -1 \leq \underbrace{1 + \frac{2\nu\Delta t}{\Delta x^2}(\cos\phi_k - 1) \leq 1}_{\text{always true}} \quad \Rightarrow \tag{9.16}$$

$$\Rightarrow \quad 2 \geq \frac{2\nu\Delta t}{\Delta x^2}(1 - \cos\phi_k) \tag{9.17}$$

For $\cos\phi_k = -1$:

$$\frac{1}{2} \geq \underbrace{\frac{\nu\Delta t}{\Delta x^2}}_{\beta} \ . \tag{9.18}$$

This is the final stability limit for the diffusion equation in one dimension,

$$\frac{\nu\Delta t}{\Delta x^2} = \beta \leq \frac{1}{2} \ . \tag{9.19}$$

We can now do a similar analysis in two dimensions using the von Neumann analysis for a central scheme.

$$\text{2D:} \qquad \frac{\partial u}{\partial t} = \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) \tag{9.20}$$

$$\frac{u_{ij}^{n+1} - u_{ij}^n}{\Delta t} = \nu \left(\frac{u_{i-1,j}^n - 2u_{ij}^n + u_{i+1,j}^n}{\Delta x^2} + \frac{u_{i,j-1}^n - 2u_{i,j}^n + u_{i,j+1}^n}{\Delta y^2} \right) \tag{9.21}$$

Since:

$$u_{ij}^n = \hat{u}_{kl}^n e^{ik\alpha x_i} e^{il\beta y_j} \ , \quad \phi_k = k\alpha\Delta x \ , \quad \phi_l = l\beta\Delta y \tag{9.22}$$

It is possible to write:

$$\hat{u}_{kl}^{n+1} = \hat{u}_{kl}^n + \frac{\nu\Delta t}{\Delta x^2}(2\cos\phi_k - 2)\hat{u}_{kl}^n + \frac{\nu\Delta t}{\Delta y^2}(2\cos\phi_l - 2)\hat{u}_{kl}^n \tag{9.23}$$

Thus:

$$\hat{G} = 1 + 2\underbrace{\frac{\nu\Delta t}{\Delta x^2}}_{\beta_x}(\cos\phi_k - 1) + 2\underbrace{\frac{\nu\Delta t}{\Delta y^2}}_{\beta_y}(\cos\phi_l - 1) \tag{9.24}$$

As above:

$$\beta_x + \beta_y \leq \frac{1}{2} \tag{9.25}$$

For $\Delta x = \Delta y \rightarrow \beta_x = \beta_y = \beta$:

$$\beta = \frac{\nu\Delta t}{\Delta x^2} \leq \frac{1}{4} \tag{9.26}$$

This result should be compared to $\beta \leq 1/2$ obtained in 1D.

10 Non-dimensionalisation

In this section, we demonstrate how to non-dimensionalise the incompressible Navier–Stokes equations for two cases; a regular case with advection velocity and length scale, and a convection-driven case (Rayleigh–Bénard convection).

10.1 Advection-driven case

Let us consider the governing incompressible Navier–Stokes equations for the case of constant density and non-uniform temperature,

$$\rho \frac{\mathrm{D}u_i}{\mathrm{D}t} = -\frac{\partial p}{\partial x_i} + \mu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + \rho f_i \ , \tag{10.27}$$

$$\rho c_p \frac{\mathrm{D}T}{\mathrm{D}t} = k \frac{\partial^2 T}{\partial x_j \partial x_j} \ , \tag{10.28}$$

$$\frac{\partial u_i}{\partial x_i} = 0 \ , \tag{10.29}$$

where the various symbols have the following dimensions:

- the velocity, u is [m/s],
- the density, ρ is [kg/m^3],
- the pressure p is [N/m^2], where N=kg m/s^2,
- the temperature T is [K],
- the dynamic viscosity μ is [N s/m^2],
- the thermal conductivity k is [W/m K], where W=kg m^2/s^3, and
- the specific heat capacity, c_p is [J/kg K].

Furthermore, it is convenient to introduce

- the kinematic viscosity,
$$\nu = \frac{\mu}{\rho} \, , \tag{10.30}$$
which is [m^2/s], and
- the thermal diffusivity,
$$\kappa = \frac{k}{\rho c_p} \, , \tag{10.31}$$
which is [m^2/s] as well.

Let us introduce characteristic (dimensional) length L_{ref}, velocity U_{ref}, density ρ_0, temperature T_{ref} and temperature difference ΔT, and non-dimensional quantities with an asteriks:

$$\begin{aligned} u_i &= u_i^* U_{\text{ref}} \ , \\ x_j &= x_j^* L_{\text{ref}} \ , \\ p &= p^* \rho U_{\text{ref}}^2 \ , \\ t &= t^* L_{\text{ref}} / U_{\text{ref}} \ , \\ \theta^* &= \frac{T - T_{\text{ref}}}{\Delta T} \quad \Rightarrow \quad T = T_{\text{ref}} + \Delta T \theta^* \\ f_i &= f_i^* U_{\text{ref}}^2 / L_{\text{ref}} \, , \end{aligned} \tag{10.32}$$

which we can employ to write the equations in non-dimensional form. The momentum equation becomes

$$\frac{\mathrm{D}u_i^*}{\mathrm{D}t^*} \cdot \frac{U_{\text{ref}}^2}{L_{\text{ref}}} = -\frac{\partial p^*}{\partial x_i^*} \cdot \frac{1}{\rho_0} \cdot \frac{1}{L_{\text{ref}}} \cdot \rho_0 U_{\text{ref}}^2 + \nu \frac{\partial^2 u_i^*}{\partial x_j^* \partial x_j^*} \cdot \frac{U_{\text{ref}}}{L_{\text{ref}}^2} + f^* \cdot \frac{U_{\text{ref}}^2}{L_{\text{ref}}}$$

and finally

$$\frac{\mathrm{D}u_i^*}{\mathrm{D}t^*} = -\frac{\partial p^*}{\partial x_i^*} + \frac{1}{Re} \frac{\partial^2 u_i^*}{\partial x_j^* \partial x_j^*} + f_i^* \, , \tag{10.33}$$

where the Reynolds number is

$$Re = \frac{U_{\text{ref}} L_{\text{ref}}}{\nu} = \frac{U_{\text{ref}}^2 / L_{\text{ref}}}{\nu U_{\text{ref}} / L_{\text{ref}}^2} = \frac{\text{advection}}{\text{viscous forces}} \, . \tag{10.34}$$

The temperature equation becomes

$$\Delta T \cdot \frac{U_{\text{ref}}}{L_{\text{ref}}} \cdot \frac{\mathrm{D}\theta^*}{\mathrm{D}t^*} = \kappa \frac{\Delta T}{L_{\text{ref}}^2} \cdot \frac{\partial^2 \theta^*}{\partial x_j^* \partial x_j^*}$$

and finally

$$\frac{\mathrm{D}\theta^*}{\mathrm{D}t^*} = \frac{1}{Pe} \frac{\partial^2 \theta}{\partial x_j^* \partial x_j^*} \, , \tag{10.35}$$

where the Péclet number is

$$Pe = Re \cdot Pr = \frac{U_{\text{ref}} L_{\text{ref}}}{\kappa} = \frac{\text{advective transport rate}}{\text{diffusive transport rate}} \, . \tag{10.36}$$

Note that the Prandtl number is a material property and defined as $Pr = \nu / \kappa$. Finally, the continuity equation becomes

$$\frac{U_{\text{ref}}}{L_{\text{ref}}} \cdot \frac{\partial u_i^*}{\partial x_i^*} = 0 \quad \Rightarrow \quad \frac{\partial u_i^*}{\partial x_i^*} = 0 \, . \tag{10.37}$$

Under this scaling, only the Prandtl number as material property (ratio of viscosity and diffusivity), and the Reynolds number as a dynamic control parameter remain.

10.2 Boussinesq approximation

Under the Boussinesq approximation, a flow with varying density can be treated using the same incompressible (constant-density) equations as in the previous section, by introducing a hydrostatic (background) pressure,

$$\frac{\partial p_0}{\partial x_i} = \rho_0 g_i \ , \tag{10.38}$$

and pressure and density fluctuations

$$p = p_0 + p' \quad \text{and} \quad \rho = \rho_0 + \rho' \, , \tag{10.39}$$

where the density variation can be expressed as function of temperature

$$\rho = \rho_0[1 - \alpha(T - T_0)] \quad \Rightarrow \quad \rho' = -\rho_0 \cdot \alpha(T - T_0) \, , \tag{10.40}$$

where α is the thermal expansion coefficient, which has unit [1/K], and T_0, ρ_0 and p_0 are reference values of temperature, density and pressure. Substituting these expression into the momentum equations, one finds

$$\rho_0 \frac{\mathrm{D}u_i}{\mathrm{D}t} = -\frac{\partial}{\partial x_i}(p_0 + p') + \mu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + \rho_0(1 - \alpha(T - T_0))g_i \ .$$

As part of the Boussinesq approximation, the density fluctuations are only retained in the bouyancy term. Subtracting the hydrostatic part and dropping the primes, we find that the forcing in the momentum equations becomes

$$f_i = -\alpha(T - T_0)g_i \ . \tag{10.41}$$

Using the above non-dimensionalisation of the forcing term, one gets

$$f_i^* = \frac{L_{\text{ref}}}{U_{\text{ref}}^2} \cdot f_i = -\frac{L_{\text{ref}}}{U_{\text{ref}}^2} \cdot \alpha(T - T_0)g_i \, . \tag{10.42}$$

This expression can be written as

$$f_i^* = -\frac{L_{\text{ref}}}{U_{\text{ref}}^2} \alpha g \Delta T \theta^* \frac{g_i}{g} = -Ri\theta^* \frac{g_i}{g} \, , \tag{10.43}$$

with the Richardson number defined as

$$Ri = \alpha g \frac{L_{\text{ref}}}{U_{\text{ref}}^2} \cdot \Delta T = \frac{\text{buoyancy}}{\text{flow shear stress}} \, . \tag{10.44}$$

10.3 Convection-driven case (Rayleigh–Bénard convection)

For a convection-driven case, we still need to define a velocity scale. Assuming similarity of diffusive and advective time scales at equilibrium, we write

$$\frac{L_{\mathrm{ref}}}{U_\kappa} = \frac{L_{\mathrm{ref}}^2}{\kappa} \quad \Rightarrow \quad U_\kappa = \frac{\kappa}{L_{\mathrm{ref}}}\,, \tag{10.45}$$

where U_κ is the convective velocity scale. In this case, the Péclet number is exactly equal to unity, yielding

$$Pe = 1\,, \quad Re = 1/Pr \quad \text{and} \quad Ri = Pr \cdot Ra\,, \tag{10.46}$$

where the Rayleigh number is defined as:

$$Ra = \alpha g L_{\mathrm{ref}}^3 \frac{\Delta T}{\nu\kappa} = \frac{g\alpha\Delta T}{\nu U_\kappa / L_{\mathrm{ref}}^2} = \frac{\text{buoyancy}}{\text{viscous forces}}\,. \tag{10.47}$$

The governing equations in non-dimensional form using the current scaling are thus,

$$\frac{\mathrm{D}u^*}{\mathrm{D}t^*} = \frac{\partial p^*}{\partial x_i^*} + Pr\frac{\partial^2 u_i^*}{\partial x_j^* \partial x_j^*} - RaPr \cdot \theta^* \frac{g_i}{|\boldsymbol{g}|} \tag{10.48}$$

$$\frac{\mathrm{D}\theta^*}{\mathrm{D}t} = \frac{\partial^2 \theta^*}{\partial x_j \partial x_j} \tag{10.49}$$

$$\frac{\partial u_i^*}{\partial x_i^*} = 0\,. \tag{10.50}$$

In this way, only the Prandtl number as a material property (ratio of viscosity and diffusivity), and the Rayleigh number as a dynamic control parameter remain.

11 Literature

Recommended literature for this course:

- Zikanov, O., Essential Computational Fluid Dynamics, Second edition, Wiley, 2019.
- Hirsch, C., Numerical Computation of Internal and External Flows: The Fundamentals of Computational Fluid Dynamics, Butterworth-Heinemann, 2007.
- Anderson, J. D., Computational Fluid Dynamics, McGraw-Hill, 1995.
- Moin, P., Fundamentals of Engineering Numerical Analysis, Cambridge University Press, 2010.