17 Conservation Form and Navier-Stokes Equations

It is often the case, when dealing with hyperbolic equations, that they can be formulated through conservation laws stating that a given quantity m (say, mass) is transported in space and time and is thus locally conserved. The resulting "*law of continuity*" leads to equations which are called **conservative**.

In general, an equation of the form

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{b} = Q$$

can be interpreted as a **conservation law** for a physical quantity, in above the density ρ, for which Q is a source and $\mathbf{b}$ is its **flux** or sometimes referred to as "**conserved flux**". Over any fixed volume V bounded by the surface ∂V, normal $\widehat{n}$,

$$\frac{d}{dt}\int_V \rho\, dV = \int_V Q\, dV - \oint_{\partial V} (\mathbf{b} \cdot \widehat{n})\, dS\ ,$$

so that the rate of increase of the physical quantity (note, mass $=$ density $\times$ volume) in V is equal to the total rate of generation within V less the amount that flows out of V across the boundary, note Fig. 17.1. In other words, a conservation law states that without **sources** or **sinks**, the rate of change of ρ in the interior volumetric space is equal to the net flux through the boundary Γ.

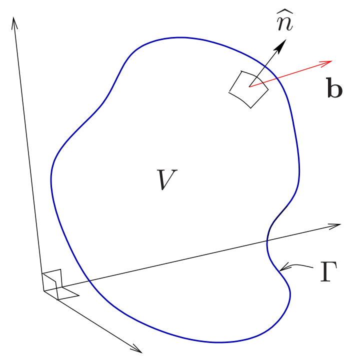

Figure 17.1: Divergence theorem.

This result, recall follows from Gauss's Divergence theorem

$$\iiint \nabla \cdot \mathbf{b}\, dV = \iint_\Gamma (\mathbf{b} \cdot \widehat{n})\, dS. \tag{17.1}$$

In a nutshell, the conserved variable ρ (say) is transported in space and time and is thus locally conserved.

17.1 Examples of conservation forms

1. Scalar conservation form:

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} f(u) = 0, \quad f(u) \ : \quad \text{flux function.} \tag{17.2}$$

   A simple example is the linear advection equation, where $f(u) = cu$. with c a constant.

2. Inviscid Burger's equation has flux

$$f(u) = \frac{1}{2}u^2.$$

3. Traffic flow equation,

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} f(\rho) = 0, \quad f(\rho) = u_m(1 - \frac{\rho}{\rho_m})\rho$$

Here the conserved variable is $\rho(x,t)$ representing density of vehicles, with $(\rho_m,\ u_m)$ parameters representing maximum density and speed.

4. In systems of conservation laws, namely

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}[\mathbf{u}]}{\partial x} = 0.$$

where trivially one may have $\mathbf{f}(\mathbf{u}) = \mathbf{A}\mathbf{u}$ with $\mathbf{A}$ the Jacobian matrix or in more complicated cases,

$$\frac{\partial \mathbf{f}[\mathbf{u}]}{\partial x} = \frac{\partial \mathbf{f}}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial x} \quad \text{with} \quad \mathbf{A} = \frac{\partial \mathbf{f}}{\partial \mathbf{u}},$$

i.e. Eqn 17.9 or Eqn. **??** (see later).

Example

Consider the following system governing *isothermal gas dynamics*

$$\frac{\partial \mathbf{u}}{\partial t} = \frac{\partial}{\partial t}\left[\begin{array}{c} \rho \\ \rho u \end{array}\right] \; ; \; \frac{\partial \mathbf{f}[\mathbf{u}]}{\partial x} = \frac{\partial}{\partial x}\left[\begin{array}{c} \rho u \\ \rho u^2 + a^2 \rho \end{array}\right] , \tag{17.3}$$

with a a positive constant valued speed of sound. We next define the conserved variables vectorially, namely $\rho = u_1$ and $\rho u = u_2$ and the above becomes

$$\frac{\partial}{\partial t}\left[\begin{array}{c} u_1 \\ u_2 \end{array}\right] + \frac{\partial}{\partial x}\left[\begin{array}{c} u_2 \\ u_2^2/u_1 + a^2 u_1 \end{array}\right] = 0 \, . \tag{17.4}$$

The corresponding Jacobian matrix is

$$\mathbf{A}(\mathbf{U}) = \frac{\partial \mathbf{f}}{\partial \mathbf{u}} = \left[\begin{array}{cc} 0 & 1 \\ -(u_2/u_1)^2 + a^2 & 2u_2/u_1 \end{array}\right] = \left[\begin{array}{cc} 0 & 1 \\ -u^2 + a^2 & 2u \end{array}\right] . \tag{17.5}$$

It is a trivial matter to show that the eigenvalues of $\mathbf{A}$ are

$$\lambda_1 = u - a \quad \text{and} \quad \lambda_2 = u + a.$$

17.2 Compressible viscous Navier-Stokes equations (NSE)

In the previous section we studied in detail the behaviour and the general solution of the simplest PDE of hyperbolic type, namely the linear advection $u_t + cu_x = 0$, with constant wave propagation speed c. We next consider more complex systems of coupled PDEs. A typical example is the system of Navier-Stokes Equations (NSEs).

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0, \tag{17.6a}$$

$$\rho\left(\frac{\partial u_j}{\partial t} + u_j \frac{\partial u_i}{\partial x_i}\right) = \nabla \cdot \Pi_{ij}, \tag{17.6b}$$

$$\rho\left(\frac{\partial h}{\partial t} + u_i \frac{\partial h}{\partial x_i}\right) - \left(\frac{\partial p}{\partial t} + u_i \frac{\partial p}{\partial x_i}\right) = \nabla \cdot (\kappa \nabla T) + \Phi, \tag{17.6c}$$

Where ρ is the mass density, u_i is the velocity vector, Π_{ij} is the stress tensor, h is the specific heat enthalpy, and $q = -\kappa \nabla T$ approximated by the Fourier law is the heat flux. Indices i, j equal $1, 2, 3$, with x_i spatial coordinates (x, y, z) say in three-dimensions and t a time variable, and repeated indices are summed over. Eqn. 17.6a expresses conservation of mass, Eqn. 17.6b expresses conservation of momentum, and Eqn. 17.6c expresses conservation of energy in which Φ is known as the viscous dissipation.

The stress tensor (Π_{ij}) and the specific enthalpy (h) are

$$\Pi_{ij} = -nk_B T\delta_{ij} - \frac{2}{3}\mu \frac{\partial u_k}{\partial x_k}\delta_{ij} + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \tag{17.7}$$

$$h = C_p T \tag{17.8}$$

Here the density $n = \rho/m$, m is the mass, T is the temperature and C_p the specific heat capacity.

17.2.1 Inviscid conservation-law (Euler) form – Ideal gas dynamics

In three space dimensions (x, y, z) neglecting viscosity and heat conduction, formulating the NSEs in conserved variables $(\rho,\ \rho u,\ \rho v,\ \rho w,\ E)^{\mathsf{T}}$, we have five inviscid conservation laws

$$\rho_t + (\rho u)_x + (\rho v)_y + (\rho w)_z = 0\ , \tag{17.9a}$$

$$(\rho u)_t + (\rho u^2 + p)_x + (\rho uv)_y + (\rho uw)_z = 0\ , \tag{17.9b}$$

$$(\rho v)_t + (\rho uv)_x + (\rho v^2 + p)_y + (\rho vw)_z = 0\ , \tag{17.9c}$$

$$(\rho w)_t + (\rho uw)_x + (\rho vw)_y + (\rho w^2 + p)_z = 0\ , \tag{17.9d}$$

$$E_t + [u(E+p)]_x + [v(E+p)]_y + [w(E+p)]_z = 0\ . \tag{17.9e}$$

Here E is the total energy per unit volume

$$E = \rho\left(\frac{1}{2}(u^2 + v^2 + w^2) + e\right), \tag{17.10}$$

and $e = C_v T$ is the specific internal energy with C_v a specific heat at constant volume. For a *gamma law gas* the pressure P is given by the equation of state

$$p = (\gamma - 1)\left(E - \frac{1}{2}\rho u^2\right), \tag{17.11}$$

with $\gamma = C_p/C_v$. The Euler equations can be shown to be hyperbolic.

The conservation laws (17.9) can be expressed in a very compact notation by defining a column vector $\mathbf{U}$ of **conserved variables** and flux vectors $\mathbf{F}(U), \mathbf{G}(U), \mathbf{H}(U)$ in the x, y and z directions, respectively. Namely:

$$\mathbf{U}_t + \mathbf{F}(U)_x + \mathbf{G}(U)_y + \mathbf{H}(U)_z = 0. \tag{17.12}$$

It is important to note that $\mathbf{F} = \mathbf{F}(U)$, $\mathbf{G} = \mathbf{G}(U)$, $\mathbf{H} = \mathbf{H}(U)$; that is, the flux vectors are functions of the conserved variable vector $\mathbf{U}$. Any set of PDEs written in this form is called a system of *conservation* laws. As partial derivatives are involved we call them a system of conservation laws in differential form. These may thus also be written in a much more compact form as follows :

$$\frac{\partial \mathbf{U}}{\partial t} + \sum_{i=1}^{3} \frac{\partial \mathbf{E}_i}{\partial x_i}, \tag{17.13}$$

Conservation Laws : To illustrate concepts, we next consider systems of 1D-PDE conservation laws of the form

$$\mathbf{U}_t + \mathbf{F}(U)_x = 0, \tag{17.14}$$

where

$$\mathbf{U} = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_m \end{bmatrix}, \quad \mathbf{F}(U) = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_m \end{bmatrix}. \tag{17.15}$$

$\mathbf{U}$ is the vector of conserved variables, $\mathbf{F} = \mathbf{F}(U)$ is the vector of fluxes and each of its components f_i is a function of the components u_j of $\mathbf{U}$.

Jacobian Matrix : The Jacobian of the flux function $\mathbf{F}(U)$ in Eqn. 17.14 is the matrix

$$\mathbf{A}(U) = \frac{\partial F}{\partial U} = \begin{bmatrix} \partial f_1/\partial u_1 & \dots & f_1/\partial u_m \\ \partial f_2/\partial u_1 & \dots & f_2/\partial u_m \\ \vdots & \vdots & \vdots \\ \partial f_m/\partial u_1 & \dots & f_m/\partial u_m \end{bmatrix}. \tag{17.16}$$

The entries a_{ij} of $\mathbf{A}(U)$ are partial derivatives of the components f_i of the vector F with respect to the components u_j of the vector of conserved variables U, that is $a_{ij} = \partial f_i/\partial u_j$. Now since we can write

$$\frac{\partial \mathbf{F}(U)}{\partial x} = \frac{\partial F}{\partial U}\frac{\partial U}{\partial x}, \tag{17.17}$$

Eqn. 17.14 becomes

$$U_t + A(U)U_x = 0. \tag{17.18}$$

Eigenvalues : The eigenvalues λ_i of a matrix A are the solutions of the characteristic polynomial

$$\| A - \lambda I \| = \det(A - \lambda I) = 0, \tag{17.19}$$

where I is the identity matrix. The eigenvalues of the coefficient matrix A of a system of Eqn. 17.14 are called the eigenvalues of the system. Physically, eigenvalues represent speeds of propagation of information. Speeds will be measured positive in the direction of increasing x and negative otherwise.

Hyperbolic System : A system of Eqn. 17.14 is said to be hyperbolic at a point (x,t) if A has m real eigenvalues $1,\ldots,m$ and a corresponding set of m linearly independent right eigenvectors $K(1),\ldots,K(m)$. The system is said to be strictly hyperbolic if the eigenvalues λ_i are all distinct. Note that strict hyperbolicity implies hyperbolicity, because real and distinct eigenvalues ensure the existence of a set of linearly independent eigenvectors. The Eqn. 17.14 is said to be elliptic at a point (x,t) if none of the eigenvalues λ_i of A are real.

17.3 Diagonalisation and characteristic variables

In order to analyse and solve the general IVP for Eqn. 17.14 it is found useful to transform the dependent variables $U(x,t)$ to a new set of dependent variables $W(x,t)$. To this end we recall the following :
Diagonalisable System : A matrix A is said to be diagonalisable if A can be expressed as

$$A = K\ \Lambda\ K^{-1} \ \text{ or } \ \Lambda = K^{-1}\ A\ K\ , \tag{17.20}$$

in terms of a diagonal matrix and a matrix K. The diagonal elements of Λ are the eigenvalues λ_i of A and the columns $K^{(i)}$ of K are the right eigenvectors of A corresponding to the eigenvalues λ_i, that is

$$\Lambda = \begin{bmatrix} \lambda_1 & \ldots & 0 \\ 0 & \ldots & 0 \\ \vdots & \vdots & \vdots \\ 0 & \ldots & \lambda_m \end{bmatrix}\ , \quad K = \left[K^{(1)},\ldots,[K^{(m)}\right]\ , \quad A\ K^{(i)} = \lambda_1\ K^{(i)} \tag{17.21}$$

A system Eqn. 17.18 is said to be diagonalisable if the coefficient matrix A is diagonalisable. Based on this concept of diagonalisation one then defines Eqn. 17.18 a hyperbolic system provided A has real eigenvalues and a diagonalisable coefficient matrix.

Characteristic variables

The existence of the inverse matrix K^{-1} makes it possible to define a new set of dependent variables $W = (w_1, w_2, \ldots, w_m)^T$ via the transformation

$$W = K^{-1}\ U \ \text{ or } \ U = K\ W\ , \tag{17.22}$$

so that the linear system Eqn. 17.18, when expressed in terms of W, becomes completely **decoupled**, in a sense to be defined. The new variables W are called characteristic variables. Next we derive the governing PDEs in terms of the characteristic variables, for which we need the partial derivatives U_t and U_x in Eqn. 17.18. Provided A is constant, K is also constant and therefore these derivatives are

$$U_t = K\ W_t\ , \ \ U_x = K\ W_x\ . \tag{17.23}$$

Direct substitution of these expressions into Eqn. 17.18 gives

$$K\ W_t + A\ K\ W_x = 0. \tag{17.24}$$

Multiplication of this equation from the left by K^{-1} and use of Eqn. 17.20 gives

$$W_t + \Lambda W_x = 0. \tag{17.25}$$

This is called the **canonical form** or **characteristic form** of Eqn. 17.18. When written in full this system becomes

$$\frac{\partial}{\partial t}\begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_m \end{bmatrix} + \begin{bmatrix} \lambda_1 & \dots & 0 \\ 0 & \dots & 0 \\ \vdots & \vdots & \vdots \\ 0 & \dots & \lambda_m \end{bmatrix}\begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_m \end{bmatrix}_x = 0 \tag{17.26}$$

Clearly the $i-$th PDE of this system is

$$\frac{\partial w_i}{\partial t} + \lambda_i \frac{\partial w_i}{\partial x} = 0, \quad i = 1, \dots, m \tag{17.27}$$

and involves the single unknown $w_i(x,t)$; the system is therefore decoupled and is identical to the linear advection equation; the characteristic speed is λ_i and there are now m characteristic curves satisfying m ODEs

$$\frac{dx}{dt} = \lambda_i \ , \quad i = 1, \dots, m. \tag{17.28}$$

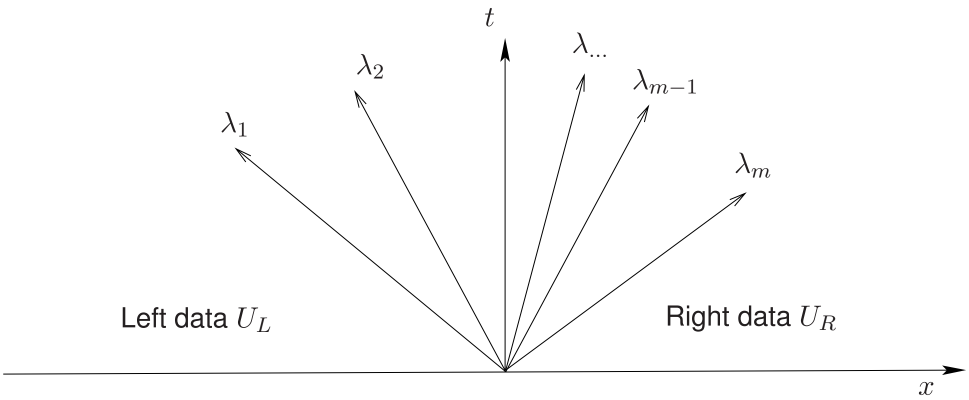

Figure 17.2: Characteristics of a linear hyperbolic system of m equations with constant coefficients.

The initial value problem

Given the initial condition,

$$\mathbf{U}^{(o)} = (u_1^{(o)}, \dots, u_m^{(o)})^{\mathsf{T}},$$

in canonical variables the initial conditions become

$$\mathbf{W}^{(o)} = K^{-1}\mathbf{U}^{(o)} \ \text{ or } \ \mathbf{U}^{(o)} = K\mathbf{W}^{(o)}.$$

Hence, each unknown $w_i(x,t)$ with corresponding initial data $w_i^{(o)}$ will be

$$w_i(x,t) = w_i^{(o)}(x - \lambda_i t), \quad i = 1, \dots, m \ . \tag{17.29}$$

Now, since

$$\mathbf{U}(x,t)=\sum_{i=1}^{m} w_i(x,t)\ \mathbf{K}^i,$$

and given Eqn. 17.29, it follows

$$\mathbf{U}(x,t)=\sum_{i=1}^{m} w_i^{(o)}(x-\lambda_i t)\ \mathbf{K}^i\ . \tag{17.30}$$

Thus the solution $\mathbf{U}(x,t)$ depends only on the initial data at the m points

$$x_o^{(i)}=x-\lambda_i t.$$

The solution 17.30 is clearly a superposition of the m waves. each of which is convected independently without change in shape; the i-th wave has shape $w_i^{(o)}(x)\ \mathbf{K}^i$ and propagates with speed λ_i.

Example

linearised equations of Gas Dynamics, see Toro (1997).

Consider the system

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix}_t+\begin{bmatrix} 0 & \rho_o \\ a^2/\rho_o & 0 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \end{bmatrix}_x=0\ ,\quad u_1\equiv\rho\ ,\quad u_2\equiv u\ , \tag{17.31}$$

where ρ_o is a constant and a^2 the speed of sound (constant too). Written in matrix form this becomes

$$U_t+A\,U_x=0. \tag{17.32}$$

The eigenvalues of A are thus given by

$$\|A-\lambda I\|=\det(A-\lambda I)=\ \det\begin{bmatrix} 0-\lambda & \rho_o \\ a^2/\rho_o & 0-\lambda \end{bmatrix}=0\ . \tag{17.33}$$

There are thus two real distinct values $\lambda_1=-a$ and $\lambda_1=+a$. The right eigenvectors $K^{(1)}$, $K^{(2)}$ are thus

$$K^{(1)}=\begin{bmatrix} \rho_o \\ -a \end{bmatrix}\ ,\quad K^{(2)}=\begin{bmatrix} \rho_o \\ a \end{bmatrix}. \tag{17.34}$$

Thus the K matrix of right eigenvectors and its inverse K^{-1} may be stated as

$$K=\begin{bmatrix} \rho_o & \rho_o \\ -a & a \end{bmatrix}\ ,\quad K^{-1}=\frac{1}{2a\rho_o}\begin{bmatrix} a & -\rho_o \\ a & \rho_o \end{bmatrix}\ . \tag{17.35}$$

Hence in terms of characteristic variables Eqn. 17.25, we may write

$$\begin{bmatrix} w_1 \\ w_2 \end{bmatrix}_t+\begin{bmatrix} -a & 0 \\ 0 & a \end{bmatrix}\begin{bmatrix} w_1 \\ w_2 \end{bmatrix}_x=0\ , \tag{17.36}$$

or in full form

$$\frac{\partial w_1}{\partial t}-a\frac{\partial w_1}{\partial x}=0\ ,\quad \frac{\partial w_2}{\partial t}+a\frac{\partial w_2}{\partial x}=0\ . \tag{17.37}$$

Given some initial condition on $U(x,0)$

$$\begin{bmatrix} w_1^{(o)} \\ w_2^{(o)} \end{bmatrix} = K^{-1} \begin{bmatrix} u_1^{(o)} \\ u_2^{(o)} \end{bmatrix} \tag{17.38}$$

written in full form

$$\begin{aligned} w_1^{(o)}(x) &= \tfrac{1}{2a\rho_o}\left[a u_1^{(o)}(x) - \rho_o u_2^{(o)}(x)\right] , \\ w_2^{(o)}(x) &= \tfrac{1}{2a\rho_o}\left[a u_1^{(o)}(x) + \rho_o u_2^{(o)}(x)\right] . \end{aligned} \tag{17.39}$$

Hence, since the solution to $(w_1,\ w_2)$, on noting Eqn. 17.37, is

$$w_1 = w_1^{(o)}(x+at) , \quad w_2 = w_2^{(o)}(x-at) , \tag{17.40}$$

it follows that the solution in characteristic variables is

$$\begin{aligned} w_1(x,t) &= \tfrac{1}{2\rho_o}\left[a u_1^{(o)}(x+at) - \rho_o u_2^{(o)}(x+at)\right] , \\ w_2(x,t) &= \tfrac{1}{2\rho_o}\left[a u_1^{(o)}(x-at) + \rho_o u_2^{(o)}(x-at)\right] . \end{aligned} \tag{17.41}$$

We may then transform the solution back to the original problem using $U = K\ W$ (see Toro, 1997).

17.4 Integral forms of conservation laws

Conservation laws may be expressed in differential and integral form. There are two reasons for considering the integral form(s) of the conservation laws and seeking solutions of PDEs in "*conserved variable*" form : (i) the derivation of the governing equations is based on physical conservation principles expressed as integral relations on control volumes; (ii) the integral formulation requires less smoothness of the solution, which allows extending the class of admissible solutions to include discontinuous solutions, *i.e.* **shocks** – mathematically we allow for **weak solutions** of the PDE : A "*weak solution*" is where the derivatives may not all exist but which is nonetheless deemed to satisfy the PDE in some sense.

In FD-methods examined so far, we have computed the solution at individual discrete points. Recall, FD-discretisation formulae are based on the assumption of functions that are smooth, and these will fail when applied to discontinuous functions.

A **non-conservative** variables based method, might give a numerical solution which appears perfectly reasonable but then upon closer inspection of results, one finds inconsistencies. These methods fail at shock-waves, giving incorrect values of the shock strength, shock speed and hence shock location.

Consider the conservation of mass equation, in one space dimension

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0. \tag{17.42}$$

This may be written, with reference to Fig. 17.3, as

$$\frac{d}{dt}\int_{x_L}^{x_R} \rho(x,t)\; dx = f(x_L,t) - f(x_R,t)\;, \tag{17.43}$$

where $f = \rho u$ is the **flux function**. We next define

$$Q(t) = \int_{x_L}^{x_R} \rho(x,t)\; dx,$$

and $Q(t)$ is the *conserved* quantity in $[x_L, x_R]$, so that $Q(t)$ only changes in time t when there is a net inflow or outflow through the **control volume** boundaries.

Thus for the complete equation we have **the first integral form I** of a conservation law :

$$\frac{d}{dt}Q(t) = F\left(U(x_L,t)\right) - F\left(U(x_R,t)\right), \tag{17.44}$$

where $F(U)$ is the flux vector.

Next integrating Eqn. 17.44 over t,

$$\int_{t_1}^{t_2} \frac{d}{dt}Q(t)\; dt = \int_{t_1}^{t_2} \left[F\left(U(x_L,t)\right) - F\left(U(x_R,t)\right)\right]\; dt, \tag{17.45}$$

the **second integral conservation law II** follows

$$Q(t_2) = Q(t_1) + \int_{t_1}^{t_2} \left[F\left(U(x_L,t)\right) - F\left(U(x_R,t)\right)\right]\; dt. \tag{17.46}$$

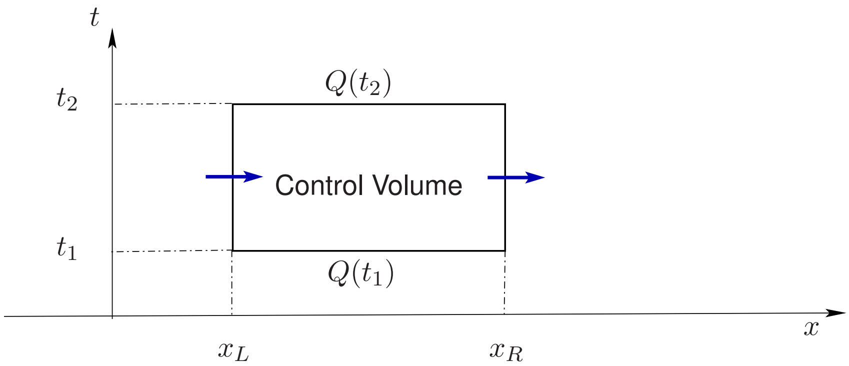

Figure 17.3: Control volume in the x, t-plane.

17.5 Finite volume conservation methods

In what follows, we divide the spatial domain into **cells of finite volume** as indicated in Fig. 17.4. We next use Eqn. 17.46 for the discrete Cell-i

$$Q_i^{n+1} - Q_i^n = \int_{t_n}^{t_{n+1}} \left[F\left(U(x_{i-1/2}, t)\right) - F\left(U(x_{i+1/2}, t)\right)\right] \, dt, \tag{17.47}$$

here we have discretised

$$Q_i^n = \int_{x_{i-1/2}}^{x_{i+1/2}} U(x, t_n) \, dx.$$

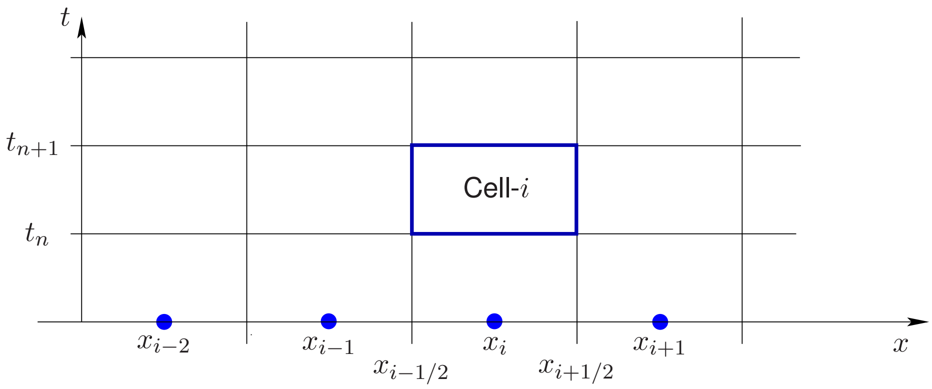

Figure 17.4: Control volume in the x, t-plane.

We can thus define

$$U_i^n = \frac{Q_i^n}{\Delta x}$$

and

$$F_{i+1/2}^{n+1/2} = \frac{1}{\Delta t}\left[\int_{t_n}^{t_{n+1}} F(U(x_{i+1/2}, t)) \, dt\right],$$

the average values of U and $F(U)$ at the interface $i + 1/2$ between t_{n+1} and t_n. Hence Eqn. 17.47 is re-written

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} + \frac{F_{i+1/2}^{n+1/2} - F_{i-1/2}^{n+1/2}}{\Delta x} = 0. \tag{17.48}$$

Note, this gives an exact formula for updating the cell average of U_i^{n+1}. On removing the superscript $(n+1/2)$ notation, summarised, we have a conservative scheme for the scalar conservation law Eqn. 17.14 or Eqn. 17.42

$$U_i^{n+1} = U_i^n + \frac{\Delta t}{\Delta x}\left[F_{i-1/2} - F_{i+1/2}\right] \ , \tag{17.49}$$

where

$$F_{i+1/2} = F_{i+1/2}\left(U_{i-l_L}, \ldots, U^n_{i+l_R}\right), \tag{17.50}$$

with l_L, l_R two non-negative integers; $F_{i+1/2}$ is called the *numerical flux function*, an approximation to the physical flux $F(U)$ in Eqn. 17.14.

Observe that Eqn. 17.49 or for that matter Eqn. 17.46 is identically equivalent to the expression

$$\oint \left[U\ dx - F(U)\ dt\right] = 0, \tag{17.51}$$

which follows from integrating Eqn. 17.14 in a domain V in $x-t$ space and using Green's theorem. The line integration along the boundary of the domain is undertaken in an anti-clockwise manner. This is called **integral form III** of the conservation laws, with the integral form II a special case where the control volume is the rectangle $[x_L, x_R] \times [t_1, t_2]$.

For greater generality, we rewrite

$$F_{i+1/2} = f^*(U_i, U_{i+1}) \quad \text{and} \quad F_{i-1/2} = f^*(U_i, U_{i-1}).$$

These expressions simply state that the flux through the interface $(i+1/2)$ can be calculated based on the state of the system in cells i and $i+1$; cells $i,\ i-1$ for the flux evaluation at interface $(i-1/2)$. In general, the time integrals on the right hand side cannot be evaluated exactly, but highly accurate numerical methods are possible, all invoking the general form

$$U_i^{n+1} = U_i^n + \frac{\Delta t}{\Delta x}\left[f^*(U_i, U_{i-1}) - f^*(U_i, U_{i+1})\right]. \tag{17.52}$$

The choice of how the flux functions $f^*(U_i, U_{i-1})$ and $f^*(U_i, U_{i+1})$ are constructed thus distinguishes between different FV methods that arise in the literature. For example in higher accuracy order discretisations, we may use more points to discretise the flux function, *i.e.*

$$F_{i+1/2} = f^*(U_i, U_{i+1}, U_{i+2}) \quad \text{or even} \quad F_{i+1/2} = f^*(U_{i-1}, U_i, U_{i+1}, U_{i+2}, \ldots, U_{i+p}).$$

For any particular choice of numerical flux $F_{i+1/2}$, *it can be shown* that a corresponding conservative scheme arises. A fundamental requirement on the numerical flux is the consistency condition

$$F_{i+1/2}(v, \ldots, v) = F(v) \ . \tag{17.53}$$

This means that if all arguments in Eqn. (17.50) are equal to v then the numerical flux is identical to the physical flux at $u = v$.

17.6 Shocks : Discontinuous solutions

We use the nonlinear inviscid burgers equations (Eqn. 17.2) to draw out the essential elements, re-stated here as an initial value problem

$$\left.\begin{aligned} &\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0, \quad f(u) = \frac{u^2}{2} \ : \ \text{the flux function} \\ &u(x,0) = u_o(x). \end{aligned}\right\} \text{IVP} \tag{17.54}$$

The characteristic speed

$$\lambda(u) = \frac{df}{du} = u,$$

and thus depends on the solution to u the conserved variable. As should be obvious, the flux function $f(u)$ plays a pivotal role in the solution, with the property of **monotonicity** of $\lambda(u)$ being important. We need to address three possibilities

1. $\lambda(u)$ is a monotone increasing function of u,

$$\frac{d\lambda(u)}{du} = f'' > 0 \quad \text{convex flux}$$

2. $\lambda(u)$ is a monotone decreasing function of u,

$$\frac{d\lambda(u)}{du} = f'' < 0 \quad \text{concave flux}$$

3. $\lambda(u)$ has extrema, for some u,

$$\frac{d\lambda(u)}{du} = f'' = 0.$$

For Burger's equation 17.54, as $\lambda'(u) = 1$, the flux is convex.

Now the characteristic curves satisfying the IVP is given by

$$\frac{dx}{dt} = \lambda(u), \quad \text{given that } x(0) = x_o,$$

while the PDE reduces to

$$\frac{du}{dt} = 0 \quad \text{along this characteristic path.}$$

It follows the value of u will be given by

$$u(x,t) = u_o(x_o) = u_o(x - \lambda[u_o(x_o)]\; t) \tag{17.55}$$

as x varies with t according to

$$x_o = x - \lambda[u_o(x_o)]\; t. \tag{17.56}$$

If u_o is constant valued, then clearly all characteristics at every x position will be oriented in an identical direction, as was the case with the simpler linear advection equation (see §15.2 and Fig. 15.2). In situations where $u_o = u_o(x)$, clearly a possibility arises of characteristics intersecting, even if smooth. Under such a scenario, one can envisage a region in the $x - t$ plane within which a family of characteristics will be intersecting – such regions are generally referred to as "*compressive*". Conversely, if the characteristic curves "*fan out*", such regions are referred to as "*expansive*". These features are illustrated in Fig. 17.5.

When $\lambda'(u) > 0$, the wave speed $\lambda(u)$ is an increasing function of u, higher values of u propagate faster than lower ones. At any compressive part of the wave, the wave speed $\lambda(u)$ is a decreasing function of x. The crest of the wave moves faster and the wave profile distorts to produce a multivalued solution for $u(x,t)$, and hence, it ultimately breaks. This progression is shown in Fig. 17.6.

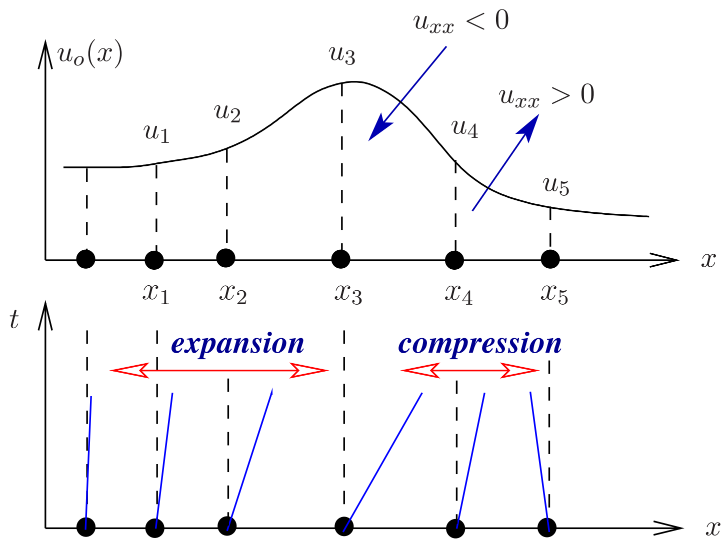

Figure 17.5: Wave steepening

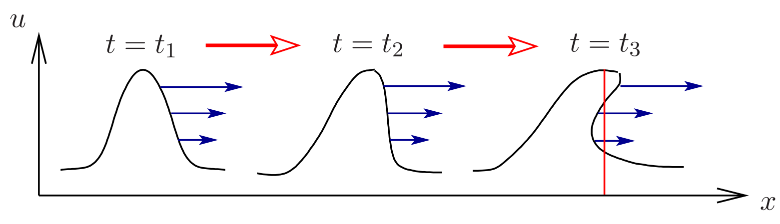

Figure 17.6: Wave profile distortion with increasing time, $t_1 < t_2 < t_3$.

17.6.1 Shock formation time

Formation of a shock arises when a family of characteristics intersect. The shock formation time is determined by evaluating the derivatives of the characteristic solutions given by Eqn. 17.55 and 17.56. Now

$$\frac{\partial u}{\partial t} = u_o' \frac{\partial x_o}{\partial t}; \quad \frac{\partial u}{\partial x} = u_o' \frac{\partial x_o}{\partial x}.$$

It follows from Eqn. 17.56

$$\frac{\partial x_o}{\partial t} = -\lambda - \lambda' u_o' \frac{\partial x_o}{\partial t}\, t, \quad \Rightarrow \quad \frac{\partial x_o}{\partial t} = \frac{-\lambda}{1 + \lambda' u_o' t}$$

while

$$\frac{\partial x_o}{\partial x} = 1 - \lambda' u_o' \frac{\partial x_o}{\partial x}\, t, \quad \Rightarrow \quad \frac{\partial x_o}{\partial x} = \frac{1}{1 + \lambda' u_o' t}.$$

These expressions thus satisfy our PDE: $u_t + \lambda u_x = 0$, **but** observe the denominator in our expressions has the possibility of being zero, *i.e.*

$$\Phi = 1 + \lambda' u_o' t.$$

For a time t for which $\Phi = 0$ we see that both $(\partial u/\partial x,\ \partial u/\partial t)$ tend to infinity – in which case a discontinuity (a shock) develops. This wave "**breaking time**" is given by

$$t_b = -\frac{1}{\lambda' u_o'}.$$

However, a smooth solution exists for all times where $\Phi \neq 0$, provided both $(\lambda',\ u_o')$ have the same signs.

17.6.2 Rankine-Hugoniot conditions and shock speed

Singularities in mathematical solutions, generally imply some weakness or shortcoming in the mathematical model of the physical phenomenon that one may be attempting to replicate. In gas dynamics, shock waves do arise, but are very narrow, *almost infinitesimally thin* regions across which very rapid **but smooth** changes occur in quantities such as pressure, temperature, density etc. over length-scales approaching the mean-free path of molecules. Thus generally, replacing the shocks waves with mathematical discontinuities is a reasonable approximation.

Consider the integral form of the conservation law (see Eqn. 17.42)

$$\frac{d}{dt}\int_{x_L}^{X_R} u(x,t)\ dx = f(u(x_L,t) - f(u(x_R,t).$$

We assume a solution $u(x,t)$ and the flux $f(u)$ and their derivatives are smooth and continuous except on a line $s = s(t)$ on the $x-t$ plane. Across $s(t)$ a jump discontinuity is imposed, and select points x_L and x_R on either sides of $s(t)$ on the x-axis. Enforcing conservation on a control volume $[x_L : x_R]$ gives

$$\frac{d}{dt}\int_{x_L}^{s(t)} u(x,t)\ dx + \frac{d}{dt}\int_{s(t)}^{X_R} u(x,t)\ dx = f(u(x_L,t) - f(u(x_R,t),$$

Recalling Leibniz's rule for differentiating under the integral, it follows

$$f(u(x_L,t) - f(u(x_R,t) = [u(s^{(-)},t) - u(s^{(+)},t)]\frac{ds}{dt} + \frac{d}{dt}\int_{x_L}^{s(t)} u_t(x,t)\ dx + \frac{d}{dt}\int_{s(t)}^{X_R} u_t(x,t)\ dx,$$

where $s^{(-)}$ is the limit as x tends to $s(t)$ from the left, and $s^{(+)}$ is the limit as x tends to $s(t)$ from the right. Next taking the limits $x_L \to s^{(-)}$ and $x_R \to s^{(+)}$ the integral terms vanish, and we obtain

$$f(u(x_L,t) - f(u(x_R,t) = [u(s^{(-)},t) - u(s^{(+)},t)]\frac{ds}{dt},$$

or in a compact form

$$[f(u)]_{+}^{-} = S[u(x,t)]_{+}^{-}. \tag{17.57}$$

Here, we have written $S = ds/dt$ the speed of the discontinuity, while expression 17.57 is called the **Rankine-Hugoniot jump condition**. Solving for the speed, it follows

$$S = \frac{\Delta f}{\Delta u},$$

where Δf and Δu are the jump values of $(f,\ u)$ on either sides of the shock. For Burger's equation, we note that

$$S = \frac{1}{2}(u_L + u_R).$$

17.6.3 On weak solutions

The notion of a solution $u(x,t)$ being analytic or at least infinitely differentiable, generally defines a smooth function. A less strict requirement, would be to ask for a solution of a PDE of order k to be at least k times differentiable. In this case, all derivatives in the equation will exist and be continuous: this is called a "**classical solution**" of the PDE.

Shock waves represent discontinuous solutions to the PDE, and integral conservation laws allow us to to obtain solutions which are not differentiable nor continuous. These solutions are called **weak** or **generalised** solutions.

To show that a weak solution of the initial value PDE problem, is acceptable (if we loosen smoothness requirements), is by way of considering a class of test functions $\phi = \phi(x,t)$ having **compact support**. An example of a compact support, would be say a rectangular region

$$\mathcal{D} = (x,t): \ a \leq x \leq b, \ \text{ and } \ 0 \leq t \leq T$$

in the (x,t)-plane, where $\phi = 0$ outside of $\mathcal{D}$.

Let us take Eqn. 17.54 factor it with $\phi(x,t)$ and integrate over the domain $\mathcal{D}$, namely

$$\iint_{\mathcal{D}} (u_t + f_x)\, \phi \; dx\; dt = 0.$$

Integrating by parts gives

$$\int_a^b \left([u\phi]_0^T - \int_0^T u\phi_t \; dt \right) \; dx + \int_o^T \left([f\phi]_a^b - \int_a^b f\phi_x \; dx \right) \; dt = 0,$$

hence

$$\int_a^b \phi(x,0) u_o(x) \; dx + \int_a^b \int_o^T u\phi_t \; dt \; dx + \int_a^b \int_o^T f\phi_x \; dt \; dx = 0.$$

Thus, for $t > 0$

$$\iint_{\mathcal{D}} (u\phi_t + f\phi_x) \; dx \; dt + \int \phi(x,0) u_o(x) \; dx = 0, \tag{17.58}$$

and this holds for all test functions $\phi(x,t)$, and importantly does not involve any derivatives of u or f : in which case this is valid even if u and f or their derivatives are discontinuous.

This shows or proves that, if $u(x,t)$ is a *classical* solution of problem 17.54, then Eqn. 17.58 holds for all test functions $\phi(x,t)$ with compact support in the (x,t)-plane. Hence, numerical solutions $u(x,t)$ or functions (even with discontinuities) which satisfy 17.58 are called the *weak* or *generalised* solutions of 17.54.

17.7 The Riemann problem

Next, we study an idealised IVP problem, the so-called Riemann problem, where u_L (left) and u_R (right) are constant valued states with a discontinuity at $x = 0$, as shown in Fig. 17.7.

$$\begin{aligned} \text{PDE :} \quad & u_t + f(u)_x = 0 \\ \text{Initial condition :} \quad & u(x,0) = u_o(x) = \begin{cases} u_L & \text{if } \ x < 0\,; \\ u_R & \text{if } \ x > 0\,. \end{cases} \end{aligned} \tag{17.59}$$

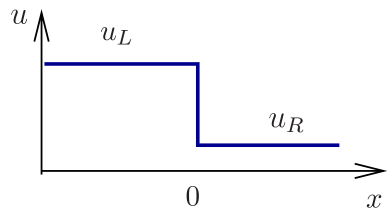

Figure 17.7: The Riemann problem

Here $u_L > u_R$, based on discussions above, it follows we expect the characteristic paths to be given by $x_L = u_L t$ and $x_R = u_R t$ on the left and right sides of the discontinuity, while where the left and right characteristics intersect a shock arises, and its path, d_S, is given by

$$d_S = \frac{1}{2}(u_L + u_R)\, t.$$

For the case, where $u_R = 0$, these key features are shown schematically in Fig. 17.8. Note the right characteristics are vertically aligned, since $dt/dx = 1/u_R$.

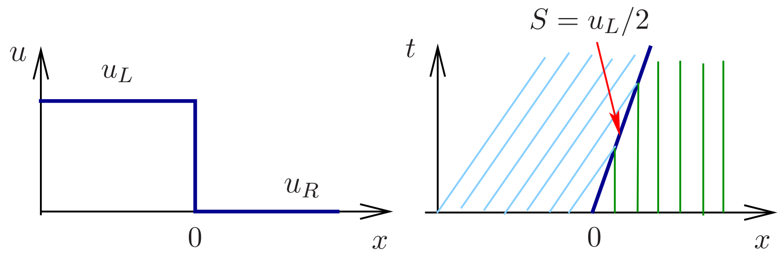

Figure 17.8: The characteristics for the shock wave

17.7.1 Entropy condition and rarefaction waves

The solution to the Riemann problem for the case, where $u_R > u_L$ and setting $u_L = 0$, namely

$$u(x,0) = \begin{cases} 0 & \text{if } \; x < 0 \\ u_R & \text{if } \; x > 0, \end{cases} \tag{17.60}$$

is shown in Fig. 17.9. In this case, the left and right characteristics do not intersect, and also a region in (x,t) space exists, into which no characteristics propagate. Amongst the many weak solutions possible, two are shown in Fig. 17.9. Both are mathematically “acceptable” weak solutions, but only the rarefaction fan solution is “physical” and thus **admissible**.

The expansion-shock solution is ruled inadmissible, through the so-called **entropy condition**[*]. The *entropy condition* is based on the requirement that characteristic curves are allowed to enter into a shock wave as in Fig. 17.8, but characteristic curves **can not emerge** from the shock. There are several variations of the entropy condition. We state only the simplest : a discontinuity propagating with speed S given by Eqn. 17.57 must satisfy the entropy condition

$$\lambda(u_L) > S > \lambda(u_R). \tag{17.61}$$

[*]to prove this is beyond the scope of this course. See Leveque *Finite Volume Methods for Hyperbolic Problems* 2002

For Burgers equation, this condition reduces to the requirement that if a discontinuity is propagating with speed S then $u_L > u_R$ – this is satisfied for the case shown in Fig. 17.8.

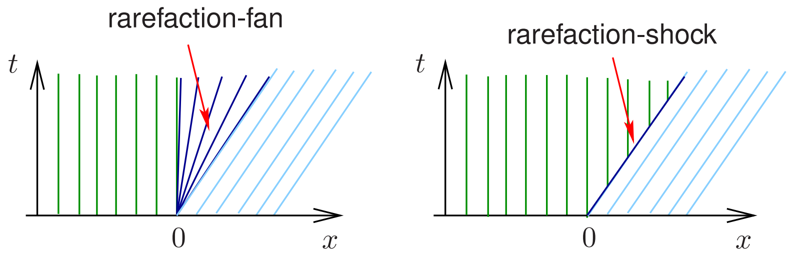

Figure 17.9: The characteristics for the rarefaction fan and the rarefaction shock (physically inadmissible).

Rarefaction shocks are called entropy-violating shocks. The connection with entropy comes from gas dynamics, and the second law of thermodynamics requiring that the entropy of a system must not decrease with time. Across a physically admissible shock the entropy of the gas increases. However across a rarefaction shock, the entropy of the gas decreases, which is inadmissible on physical grounds and therefore rejected.

For completeness, the expansion-fan solution, where $u_L = 0$, is

$$u(x,t) = \begin{cases} 0 & \text{if } \; x < 0, \\ x/(u_R\, t) & \text{if } \; 0 < x/u_R \leq t, \\ u_R & \text{if } \; x/u_R > t. \end{cases} \tag{17.62}$$

Expansive smooth initial data

An alternative means to see why the expansion fan is the correct solution to impose, is to consider the scenario shown in Fig. 17.10, where a linear variation in $u_o(x)$ is prescribed separating the left and right constant valued states $(u_L,\ u_R)$ by the distance $\Delta x = c - a$. In this case, we can clearly see that an expansion fan arises, which “smoothly” connects the left and right states.

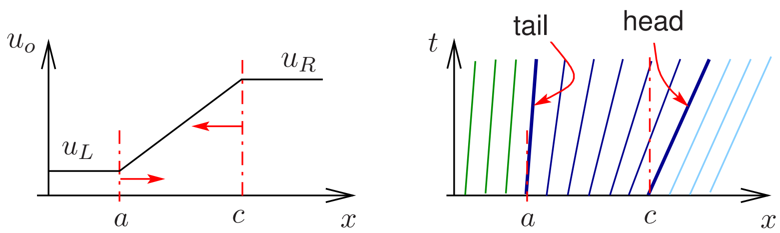

Figure 17.10: The characteristics for the rarefaction fan.

Next imagine $\Delta x \to 0$, *i.e.* points a, c coinciding. No matter how small the Δx interval is, the structure of the above expansion fan solution remains unaltered and is entirely different from the expansion-shock solution, for which small changes to the data lead to large changes in the solution – which if you recall is an undesirable property.

17.8 Riemann Solution for the inviscid Burgers equation

At an interface $x = 0$, we pose a Riemann problem :

$$u(x, t = 0) = \begin{cases} u_i^n & u_L \quad \text{if } \; x < 0 \;; \\ u_{i+1}^n & u_R \quad \text{if } \; x > 0 \;. \end{cases} \tag{17.63}$$

Observe that this initial condition has no intrinsic length scale. If we rescale space by a factor and time by the same factor we get the same solution. It follows that

$$u(x, t) = u(x/t).$$

This means in particular that

$$u(x = 0, t) = u(x/t = 0) = constant,$$

hence,

$$u_{Riemann}(x = 0, t) = u(u_L, u_R), \quad \text{for } \; t^j \leq t \leq t^{j+1}.$$

In summary, solutions of the Riemann problem for Burgers equation, are as follows

$$\begin{aligned} \text{PDE :} \quad & u_t + u u_x = 0 \\ \text{Initial condition :} \quad & u(x, 0) = u_o(x) = \begin{cases} u_L & \text{if } \; x < 0 \;; \\ u_R & \text{if } \; x > 0 \;. \end{cases} \end{aligned} \tag{17.64}$$

We have the possibility of a simple wave emanating from the origin $x = 0$, a shock wave if $u_L > u_R$, or an expansion wave when $u_L < u_R$. The solution summarised is

1. For $u_L > u_R$: the solution is a shock wave, with shock speed $S = (u_L + u_R)/2$

$$u(x, t) = \begin{cases} u_L & \text{if } \; x - S\,t < 0 \\ u_R & \text{if } \; x - S\,t > 0. \end{cases} \tag{17.65}$$

2. For $u_L < u_R$: the solution is a rarefaction wave

$$u(x, t) = \begin{cases} u_L & \text{if } \; x/t \; < u_L \\ x/t & \text{if } \; u_L < x/t < u_R \\ u_R & \text{if } \; x/t \; > u_R. \end{cases} \tag{17.66}$$