

Chapter 2

Transport Equations

Many systems exhibit evolution over time with properties of interest that vary throughout their spatial domains. Examples of such systems arise in *population dynamics*, which describes the distribution of individuals in some population and how they interact. “Individuals” could refer to molecules, electrons, particles, animals, people, company stocks, or network messages.

One way to study the overall population is to attempt to track each individual, such approaches are sometimes called *individual-based models*. The tracking process is usually very labour intensive and involves collecting a lot of data on the actions of all individuals. If this level of detail is not crucial and a more ‘large-scale’ view is of interest, then *continuum theory* may be a better option.

Continuum theories yield evolution equations with respect to properties that are averaged over small intervals of time and small regions of space. In such cases, we implicitly assume a *continuum hypothesis* which states that appropriately averaged behaviours of individuals can be generally predicted from trends in the local population. We consequently formulate *continuum models* as partial differential equations (PDE) governing the evolution of density functions ($f(\mathbf{x}, t)$) describing properties of the population at a given position and time. Integrating the density over the entire domain can be used to capture the time-dependence of the property on the whole population, $\mathcal{F}(t) = \int f(\mathbf{x}, t) d\mathbf{x}$.

Some specific applications of continuum models include:

- Fluid dynamics: the flow of liquids and gases (density of molecules in space)
- Solid mechanics: the deformation of solids (density of molecules in space)
- Electromagnetics: the flow of electric currents in materials (density of electric charges in space)
- Scattering theory: dynamics due to collisions in high energy particle physics (density of particles having different velocities)

- Age-structured population dynamics: birth, death, and aging of a population (distribution of individuals having different ages) [28, 74]
- Size-structured population dynamics: growth and decay of physical sizes of individuals in a population (distribution of individuals having different sizes) [8]

Fluid dynamics and solid mechanics are often grouped together under the heading of *continuum mechanics*. Other population models focus not on change in position, but on properties like stock price in financial models, popularity in social networks or genetic traits in biological systems.

In each of these contexts, PDEs can be used to describe the redistribution of the property of interest over time. Conveying shifts or “motion” in the density, whether with respect to spatial position or with the independent variable \mathbf{x} representing other properties (e.g. velocity, age, size), such PDEs are also broadly called *transport equations*. The common structure shared by these models is having a PDE for the rate of change of the density involving the spatial gradient of a *flux function*, which characterises transport of the property within the population. Transport equations are fundamental for describing problems in many fields extending from theoretical physics, chemical engineering, and mathematical biology to probability theory.

In this chapter we introduce the fundamental approach for formulating transport models (conservation laws and the Reynolds transport theorem). We then go on to describe the method of characteristics, a methodology for constructing exact solutions to basic transport models.

2.1 The Reynolds Transport Theorem

As a conceptual starting point, we consider how we might describe the dynamics of individuals in a large population—describing their motion (change of absolute position as a function of time, $\mathbf{X}(t)$) and deformation (rearrangement or change of relative position within groups of surrounding individuals).

In order to introduce the basic principles, we begin by studying the case of *passive transport* of inert particles carried by an externally imposed flow field, for example, particles of dust cloud in the wind or a pollutant carried in a running river. Here “passive” indicates that the presence of the particles does not influence the flow driving their motion.

Each particle can be uniquely identified by its initial position at time $t = 0$,

$$\mathbf{X}(t = 0) = \mathbf{A} = (A, B, C) \quad (X(t = 0) = A \text{ in 1D }) \quad (2.1a)$$

Assume an imposed velocity field, $\mathbf{v}(\mathbf{x}, t)$, is given that specifies the speed and direction that a particle occupying position \mathbf{x} would take at time t . Having an explicit expression for properties in a fixed coordinate system is called an *Eulerian description*. From the definition of velocity as the rate of change of position, the motion of a particle is given by

$$\frac{d\mathbf{X}}{dt} = \mathbf{v}(\mathbf{X}, t), \quad \left(\frac{dX}{dt} = v(X, t) \text{ in 1D} \right) \quad (2.1b)$$

This initial value problem gives the motion of a particle over time, and is sometimes called the problem for the particle's *pathline*.

An alternative point of view is to recognise that for a particle starting from position (2.1a), the Eulerian description of the entire velocity field is not needed. All that is essential is the velocity along the particle's pathline. The *Lagrangian description* gives a property following the motion of a given particle as a function of time. The Lagrangian velocity for the particle starting from position \mathbf{A} is

$$\mathbf{V}(t; \mathbf{A}) = \mathbf{v}(\mathbf{X}(t; \mathbf{A}), t). \quad (2.2)$$

The problem for the pathline can then be restated in Lagrangian form as

$$\frac{d\mathbf{X}}{dt} = \mathbf{V}(t; \mathbf{A}), \quad \mathbf{X}(0; \mathbf{A}) = \mathbf{A}. \quad (2.3)$$

We will show that the ability to change between these two equivalent forms will enable us to solve transport equations.

Values of other properties carried by point particles (e.g. density, temperature, radioactivity) can similarly be expressed in both Eulerian $f(\mathbf{x}, t)$ and Lagrangian $F(t)$ forms via

$$F(t; \mathbf{A}) = f(\mathbf{X}(t; \mathbf{A}), t). \quad (2.4)$$

In describing the evolution of any property f following a particular particle, it is necessary to calculate the rate of change of f for the given particle $f_{\text{part}}(t) \equiv F(t; \mathbf{A}) = f(\mathbf{X}(t; \mathbf{A}), t)$. Using the chain rule, we can express this ‘‘Lagrangian time derivative’’ in terms of Eulerian functions,

$$\begin{aligned} \frac{df_{\text{part}}}{dt} &= \frac{\partial f}{\partial t} + \nabla f \cdot \frac{d\mathbf{X}}{dt} \\ &= \boxed{\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f \equiv \frac{Df}{Dt}} \end{aligned} \quad (2.5)$$

where we have used (2.1b). The Eulerian form of this derivative is called the *convective (or material) derivative* and is denoted $\frac{Df}{Dt}$. We will see that the velocity field defining the flow has a special role in transport equations. If \mathbf{v} is given, then the problem for the evolution of the property of interest is called a *kinematics problem* (as in passive transport). If the evolution of \mathbf{v} is coupled to f and must be determined as part of the solution, then it is a more challenging *dynamics problem*.

The next stage in formulating a continuum model is to determine the rate of change of a property evaluated over a ‘‘material blob’’—in other words, we consider a specific set of particles, defined as starting from a set of \mathbf{A} values (2.1a) occupying a region D in space. For example, picture the blob as the fluid in a small droplet. The

cumulative value of property f over the material blob is given by

$$f_{\text{blob}}(t) = \iiint_{D(t)} f(\mathbf{x}, t) dV, \quad (2.6)$$

where $D(t)$ is the region occupied by the moving, deforming blob at time t . We would like to know how $f_{\text{blob}}(t)$ varies with time. In one dimension, a “blob” is simply a time-dependent interval, $a(t) \leq x \leq b(t)$ and (2.6) reduces to

$$f_{\text{blob}}(t) = \int_{a(t)}^{b(t)} f(x, t) dx. \quad (2.7)$$

To find the rate of change, we apply Leibniz’s rule to determine the derivative of an integral with time-dependent endpoints,

$$\begin{aligned} \frac{d}{dt} \left(\int_{a(t)}^{b(t)} f(x, t) dx \right) &= \int_a^b \frac{\partial f}{\partial t} dx + \underbrace{f(b, t) \frac{db}{dt} - f(a, t) \frac{da}{dt}}_{f(x, t) \frac{dx}{dt} \Big|_{x=a}^{x=b}} \\ &= \int_a^b \left[\frac{\partial f}{\partial t} + \frac{\partial}{\partial x} \left(f(x, t) \frac{dx}{dt} \right) \right] dx \\ &= \int_a^b \left[\frac{\partial f}{\partial t} + \frac{\partial}{\partial x} (f v) \right] dx \end{aligned} \quad (2.8)$$

where again, we have made use of (the one-dimensional version) of (2.1b). In two and three dimensions, making use of the divergence theorem, we can generalise this result to give the *Reynolds Transport Theorem* [1],

$$\boxed{\frac{d}{dt} \left(\iiint_{D(t)} f dV \right) = \iiint_{D(t)} \left[\frac{\partial f}{\partial t} + \nabla \cdot (f \mathbf{v}) \right] dV} \quad (2.9)$$

2.2 Deriving Conservation Laws

In order to apply the Reynolds transport theorem to obtain a transport model, we need the introduction of a *conservation principle*. This is a statement providing information about the rate of change of f_{blob} that applies to *all possible material blobs*.

For example, requiring *conservation of mass*—the principle that total mass can be neither created nor destroyed, the mass of every blob must remain constant in time.

Expressing the mass in terms of the material density, $f \equiv \rho$, in one-dimension this gives

$$m_{\text{blob}}(t) = \int_{a(t)}^{b(t)} \rho(x, t) dx, \quad \frac{dm_{\text{blob}}}{dt} = 0 \quad \forall(a, b). \quad (2.10)$$

In order to change from a statement about properties of blobs to a transport PDE, the final tool involved is an integral result from analysis, sometimes called the *du Bois-Reymond lemma* [49], which we state in its simplest form on the one-dimensional domain $0 \leq x \leq 1$ as

$$\text{If } \int_a^b g(x) dx = 0 \quad 0 \leq \boxed{\forall(a, b)} \leq 1, \quad \text{then } \boxed{g(x) \equiv 0 \text{ for } 0 \leq x \leq 1}. \quad (2.11)$$

In other words, if an integral vanishes for all choices of sub-domains, then the integrand must vanish on the whole domain.¹ This result allows us to convert from an integral equation (called a *weak form*, applying on the domain as a whole) to a differential equation (called a *strong form* that applies locally, pointwise at each x in the whole domain), if the integral is valid for all blobs.

Applying the Reynolds Transport theorem to (2.10), we reduce the principle of conservation of mass to a PDE for the density, yielding the (local) *conservation law* for mass density in one dimension,

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v) = 0, \quad (2.12)$$

also known as the *continuity equation*. In three dimensions, the corresponding result is

$$\frac{d}{dt} \left(\iiint_{D(t)} \rho(\mathbf{x}, t) dV \right) = 0 \quad \forall D \quad \implies \quad \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0. \quad (2.13)$$

The quantity in the parenthesis is called the *flux*, \mathbf{q} , and corresponds physically to the rate of ρ passing through a fixed point per unit time (here $\mathbf{q} = \rho \mathbf{v}$).

If we are given information on the rate at which the property of interest is created or destroyed, say due to a chemical reaction as in $d\rho/dt = R$ like (1.8), then the rate of change of the total amount of the chemical in domain D be can expressed by

$$\frac{d}{dt} \left(\iiint_D \rho dV \right) = \iiint_D R dV. \quad (2.14)$$

This should be true in any subdomain (any material blob). If transport is present then $D = D(t)$ and after applying the Reynolds Transport Theorem to the left integral, we can regroup the resulting integrals together as

¹Assuming the integrand to be a smooth function.

$$\iiint_{D(t)} \left[\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) - R \right] dV = 0 \quad \forall D(t). \quad (2.15)$$

Then applying the du Bois-Reymond lemma yields the general conservation law including reaction terms (sometimes called *source* or *sink* terms depending on whether the rate of production is positive or negative),

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = R. \quad (2.16)$$

Equation (2.14) can be applied to Newton's second law, stating that the rate of change of momentum is equal to the sum of the applied forces

$$\frac{d}{dt} \left(\iiint_{D(t)} \rho \mathbf{v} dV \right) = \iiint_{D(t)} \mathbf{f} dV, \quad (2.17)$$

where \mathbf{f} gives net forces per unit volume. Applying the Reynolds transport theorem, the du Bois Reymond lemma, and expressing the forces in terms of the divergence of a stress tensor, $\mathbf{f} = \nabla \cdot \sigma$, yields the *Cauchy momentum equation*,

$$\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = \nabla \cdot \sigma. \quad (2.18)$$

Encapsulating the principles of conservation of mass and momentum, equations (2.13) and (2.18) are the basis of continuum mechanics [41, 50]. Supplemented by appropriate equations for defining the stress in terms of ρ and \mathbf{v} , called *constitutive relations* or *equations of state*, these yield the governing equations for solid mechanics and the Navier–Stokes equations for fluid dynamics.

2.3 The Linear Advection Equation

In this section we will focus on the most fundamental case of (2.16), where $R = 0$ (no reactions) and the velocity is a uniform constant vector, $\mathbf{v} = c \hat{\mathbf{i}}$ (constant speed), yielding the one-dimensional *advection equation*

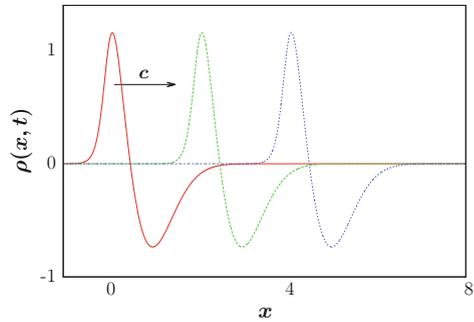
$$\frac{\partial \rho}{\partial t} + c \frac{\partial \rho}{\partial x} = 0. \quad (2.19)$$

All solutions of the advection equation can be written as constant profile *travelling waves*,

$$\rho(x, t) = P(x - ct), \quad (2.20)$$

where the terminology “travelling wave” refers to a solution moving with a fixed velocity (speed in one dimension) and with a “constant profile” meaning that the

Fig. 2.1 A travelling wave solution (2.20), $\rho(x, t) = P(x - ct)$, of (2.19) for $c > 0$ at three successive times



wave shape $P(x)$ given at $t = 0$ is maintained for all times. If $c > 0$, the wave profile propagates to the right (and to the left if $c < 0$) (see Fig. 2.1).

While (2.20) is a solution of equation (2.19) for any function P , for the purpose of considering the complexities associated with more general transport models (with other forms of flux), it is helpful to first understand the action of the equation on simple functions. If we can express $P(x)$ as a complex Fourier series (see Appendix A), $P(x) = \sum_k A_k e^{ikx}$, then the travelling wave (2.20) can be written as

$$\rho(x, t) = \sum_{k=-\infty}^{\infty} A_k e^{ik(x-ct)} = \sum_{k=-\infty}^{\infty} A_k e^{i[kx - \omega t]}, \quad (2.21)$$

where k is called the wave number (related to the wavelength between successive crests of $\cos(kx)$ in space, $L = 2\pi/k$) and ω is called the angular frequency (related to the period of oscillation of $\sin(\omega t)$ in time, $T = 2\pi/\omega$). For (2.19), the expansion (2.21) defines $\omega = ck$, but the Fourier decomposition is applicable to other equations as long as a relationship can be found between the frequency and the wavenumber, $\omega = \omega(k)$, called the *dispersion relation*.

Consider the fifth order linear homogeneous constant-coefficient PDE

$$\frac{\partial \rho}{\partial t} + c_1 \frac{\partial \rho}{\partial x} + c_3 \frac{\partial^3 \rho}{\partial x^3} + c_5 \frac{\partial^5 \rho}{\partial x^5} = 0. \quad (2.22)$$

If we substitute in a Fourier mode $\rho_k(x, t) = A_k \exp(i[kx - \omega t])$ (called a *uniform plane wave*) as a trial solution, (2.22) reduces to a relationship between ω and k given by

$$-i\omega + c_1(ik) + c_3(ik)^3 + c_5(ik)^5 = 0,$$

which determines the dispersion relation, $\omega(k) = c_1 k - c_3 k^3 + c_5 k^5$.

Descriptions of wave properties in terms of the dispersion relation are fundamental in many models that arise as generalisations of the advection equation. The *phase speed*, $c_p(k) \equiv \omega(k)/k$, gives the speed of waves with wavenumber k . Equation (2.19) has constant phase speed (being independent of k), and so is called *dispersionless*

because all of its wave modes travel at the same speed, maintaining the steady profile $P(x - ct)$ (2.21). In contrast, for *dispersive* equations with $c_p(k) \neq \text{constant}$, the profile given by the sum $\rho(x, t) = \sum_k A_k e^{ik[x - c_p(k)t]}$ changes with time as the component waves separate (“disperse”) according to their different speeds. The growth or decay of waves is described by dispersion relations having imaginary components: wave amplitudes are maintained if $\omega(k)$ is purely real, while if $\omega(k)$ has an imaginary part then *dissipation* occurs. In order to observe this effect, consider what happens when we substitute the plane wave solution into the diffusion equation $\rho_t = \rho_{xx}$; the dispersion relation is found to be $\omega = -ik^2$, so that the (real-valued) phase speed is $c_p = 0$ and the wave will dissipate without propagating: $\rho_k(x, t) = (A_k e^{-k^2 t}) e^{ikx}$ (these correspond to so-called ‘standing waves’).

We now turn our attention to describing methods for obtaining the solutions to various generalisations of the advection equation (2.19).

2.4 Systems of Linear Advection Equations

Consider a system of two coupled linear advection equations for properties $p(x, t)$, $q(x, t)$ on $-\infty < x < \infty$,

$$p_t + ap_x + bq_x = 0 \quad (2.23a)$$

$$q_t + cp_x + dq_x = 0 \quad (2.23b)$$

where a, b, c, d are constants, and the initial conditions are given by

$$p(x, 0) = f(x) \quad q(x, 0) = g(x). \quad (2.23c)$$

The typical approach for determining the solutions of (2.23) is to decouple the system into independent advection equations, each with a travelling wave solution of the form

$$\frac{\partial w}{\partial t} + \lambda \frac{\partial w}{\partial x} = 0 \quad \Rightarrow \quad w(x, t) = W(x - \lambda t), \quad (2.24)$$

where λ is the wave speed for some appropriate travelling wave profile W .

We start by assuming a solution as a linear combination,

$$w(x, t) = Ap(x, t) + Bq(x, t), \quad (2.25)$$

for some constants A, B to be determined. Forming the linear combination of $A \cdot$ (2.23a) + $B \cdot$ (2.23b) yields

$$(Ap + Bq)_t + (aA + cB)p_x + (bA + dB)q_x = 0,$$

while substituting w from (2.25) into (2.24) gives

$$(Ap + Bq)_t + (\lambda A)p_x + (\lambda B)q_x = 0.$$

Comparing coefficients in these equations leads to a matrix eigenvalue problem,

$$\begin{pmatrix} a & c \\ b & d \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \lambda \begin{pmatrix} A \\ B \end{pmatrix}. \quad (2.26)$$

Solving this system yields the eigenvalues (λ) defining the wave speeds and the components of the eigenvectors defining the relationship of w to the solutions p and q , (2.25). In order for the eigenvalues to be meaningful as speeds, they must be real values. The solutions of the eigenvalue problem, λ_1 and A_1, B_1 , and λ_2 and A_2, B_2 , determine the travelling wave solutions

$$\begin{aligned} w_1(x, t) &= A_1 p(x, t) + B_1 q(x, t) = W_1(x - \lambda_1 t), \\ w_2(x, t) &= A_2 p(x, t) + B_2 q(x, t) = W_2(x - \lambda_2 t), \end{aligned} \quad (2.27)$$

where the travelling wave profiles $W_1(x), W_2(x)$ are otherwise undetermined so far. Applying initial conditions (2.23c) to evaluate these equations at time $t = 0$ explicitly defines the wave profiles as satisfying

$$\begin{aligned} A_1 f(x) + B_1 g(x) &= W_1(x), \\ A_2 f(x) + B_2 g(x) &= W_2(x). \end{aligned} \quad (2.28)$$

With W_k now known in terms of f, g and the A_k, B_k coefficients given by the eigenvectors, the right-hand side of (2.27) is known, yielding a linear system for $p(x, t), q(x, t)$ in terms of combinations of $f(x - \lambda_k t)$ and $g(x - \lambda_k t)$ (with $k = 1, 2$).

This approach extends to systems of any number of coupled linear equations,

$$\frac{\partial \mathbf{p}}{\partial t} + \mathbf{M} \frac{\partial \mathbf{p}}{\partial x} = \mathbf{0} \quad (2.29)$$

where $\mathbf{p} = (p, q, r, \dots)^T \in \mathbb{R}^n$ and \mathbf{M} is an $n \times n$ constant coefficient matrix. Assuming trial solutions of the form $w = \mathbf{u} \cdot \mathbf{p}$ where $\mathbf{u} = (A, B, C, \dots)^T$ and noting the relationship between (2.26) and the coefficients in (2.23), we see that the general eigenvalue problem can be stated as

$$\mathbf{M}^T \mathbf{u} = \lambda \mathbf{u}. \quad (2.30)$$

If all the eigenvalues of \mathbf{M}^T are real and there is a complete set of eigenvectors, then (2.29) is called a *hyperbolic system* and its solutions can be expressed in terms of sums of travelling waves (see [65, 80, 81, 106] for more details).

2.5 The Method of Characteristics

Semilinear wave equations take the form

$$\frac{\partial p}{\partial t} + c(x, t) \frac{\partial p}{\partial x} = r(x, t, p), \quad (2.31a)$$

where the speed c depends on both position and time, but not on the solution itself, and the reaction rate can depend on all three, but not on derivatives of the solution. The terminology ‘semilinear’ arises because the left-hand side of the equation is linear with respect to the dependent variable p , while the right-hand side can be nonlinear in p . Problems for this class of equations with initial conditions

$$p(x, 0) = f(x), \quad (2.31b)$$

can be solved by converting from the original Eulerian PDE form into a Lagrangian form that can be solved as a set of coupled ODEs.

In order to see how (2.31a) defines a property evolving in a flow, let the Lagrangian form of the solution for each initial material coordinate A be written as

$$P(t; A) = p(X(t; A), t) \quad X(0; A) = A. \quad (2.32)$$

Using the chain rule, the rate of change of P is

$$\frac{dP}{dt} = \frac{\partial p}{\partial t} + \frac{\partial p}{\partial x} \frac{dX}{dt} \quad (2.33)$$

and this can be matched term by term with the PDE (2.31a) if the Lagrangian variables evolve according to the *characteristic equations*

$$\frac{dP}{dt} = r(X(t), t, P(t)), \quad \frac{dX}{dt} = c(X(t), t). \quad (2.34a)$$

The initial conditions (2.31b) take the corresponding form

$$P(0; A) = f(A), \quad X(0; A) = A. \quad (2.34b)$$

The solution of the X -equation subject to its initial condition therefore defines a path in the (x, t) plane known as a *characteristic curve* (or simply a ‘characteristic’), and generalises the concept of a pathline. Once $X(t)$ has been determined, it can be substituted into the evolution equation for P (2.34a)₁ and can then be solved for $P(t)$.

Thus, the so-called *method of characteristics* replaces the Eulerian PDE with an initial value problem for a pair of ODEs. The Lagrangian solutions $(X(t; A), P(t; A))$ are parameterised by the initial material coordinate A and can sometimes be inverted to give the explicit Eulerian solution $p(x, t)$.

As an example, consider the transport problem for $p(x, t)$,

$$\frac{\partial p}{\partial t} + 2x \frac{\partial p}{\partial x} = xp^2, \quad p(x, 0) = 2 + \sin(x). \tag{2.35}$$

Following the above analysis, the corresponding characteristic problem is given by

$$\frac{dX}{dt} = 2X, \quad X(0) = A, \tag{2.36a}$$

$$\frac{dP}{dt} = XP^2, \quad P(0) = 2 + \sin(A). \tag{2.36b}$$

Solving (2.36a) yields $X(t; A) = Ae^{2t}$, which we can then substitute into the ODE for P (2.36b) to obtain the general solution

$$\frac{dP}{dt} = Ae^{2t}P^2 \quad \Rightarrow \quad P(t) = \frac{1}{C - \frac{1}{2}Ae^{2t}}.$$

Imposing the initial condition on P at $t = 0$ (when $X = A$) then yields that

$$P(t; A) = \left(\frac{A}{2} (1 - e^{2t}) + \frac{1}{2 + \sin(A)} \right)^{-1},$$

(see Fig. 2.2). Inverting $Ae^{2t} = X = x$ gives $A = xe^{-2t}$. Substituting this into $P(t; A)$ and applying $P = p$ results in the final form of the solution

$$p(x, t) = \left(\frac{x}{2} (e^{-2t} - 1) + \frac{1}{2 + \sin(xe^{-2t})} \right)^{-1}.$$

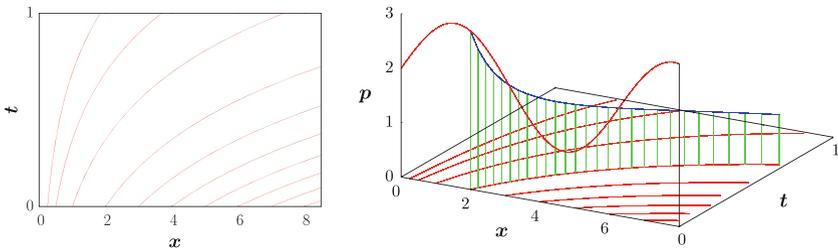


Fig. 2.2 (Left) Characteristic curves in the (x, t) plane for problem (2.35). (Right) Function values evolving on a characteristic curve

2.6 Shocks in Quasilinear Equations

Quasilinear equations differ from semilinear equations only in having the speed c depend additionally on the solution,

$$\frac{\partial p}{\partial t} + c(x, t, p) \frac{\partial p}{\partial x} = r(x, t, p). \quad (2.37)$$

This makes the characteristic ODEs fully coupled,

$$\frac{dP}{dt} = r(X, t, P), \quad \frac{dX}{dt} = c(X, t, P). \quad (2.38)$$

For semilinear equations, the equation (2.34a) for the characteristic curves $x = X(t; A)$ decouples from P , and standard existence and uniqueness results guarantee that two curves starting from different initial positions (and having different values of $P(t)$) will never intersect. This is not the case for the coupled equations in (2.38), where characteristics can cross and hence predict several different $P(t; A_j)$ values occurring simultaneously at the same x position.

As an example, consider the *inviscid Burgers equation*,

$$\frac{\partial p}{\partial t} + p \frac{\partial p}{\partial x} = 0, \quad (2.39)$$

with initial conditions

$$p(x, 0) = \begin{cases} 1 - |x| & |x| \leq 1, \\ 0 & \text{otherwise.} \end{cases} \quad (2.40)$$

Equation (2.39) is an important mathematical model that will arise again later in other contexts; one aspect of its importance can be observed by noting that if the property p is the flow velocity, then (2.39) is the convective derivative of the velocity (2.5) (the Lagrangian form of the acceleration), $\frac{Dv}{Dt} = v_t + vv_x = 0$.

The characteristic equations for this example are

$$\frac{dX}{dt} = P, \quad X(0; A) = A, \quad (2.41a)$$

$$\frac{dP}{dt} = 0, \quad P(0; A) = \begin{cases} 1 - |A| & |A| \leq 1, \\ 0 & \text{else.} \end{cases} \quad (2.41b)$$

We note that for this problem P remains constant along each characteristic, so that $X = Pt + A$ and the solution can be expressed as

$$\begin{cases} X = A, & P = 0 & A < -1, \\ X = (1 + A)t + A, & P = 1 + A & -1 \leq A \leq 0, \\ X = (1 - A)t + A, & P = 1 - A & 0 \leq A \leq 1, \\ X = A, & P = 0 & A > 1 \end{cases} \quad (2.42)$$

and restated in an explicit form for $t \geq 0$

$$p(x, t) = \begin{cases} 0 & x < -1, \\ (1 + x)/(1 + t) & -1 \leq x \leq t, \\ (1 - x)/(1 - t) & t \leq x \leq 1, \\ 0 & x > 1. \end{cases} \quad (2.43)$$

There are several points to note about this representation of the solution—first, the piecewise-defined solutions are not mutually exclusive for $t > 1$. Consequently multiple values are being predicted for p at some locations when $t > 1$. In relation to this, the third subcase becomes undefined at time $t = 1$, changing from negative slopes for $t < 1$ to positive slopes for $t > 1$. Figure 2.3 shows the characteristic curves and $p(x, t)$ profiles given by (2.43). We observe that the portion of the solution starting from $x \in [-1, 0]$ spreads out over an increasingly large region as its characteristics separate from each other (this is sometimes called an *expansion fan* or *rarefaction wave*).

In contrast, the portion of the solution starting from $x \in [0, 1]$ is being compressed into a smaller region (up until $t = 1$) and is referred to as a *compressive wave*. Its slope steepens and overturns for $t > 1$ to yield what could be described as a multi-valued “*breaking wave*”.

Mathematically this part of the solution is predicting three values for a physical quantity (maybe a density, concentration or temperature, for example) that should have a unique value at any point x at a given time t .

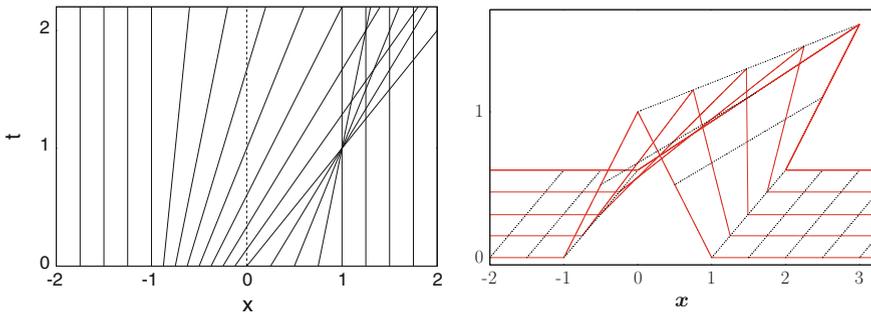


Fig. 2.3 (Left) characteristic curves $X(t; A)$ given by (2.42) in the xt plane and a 3D view of the evolving multi-valued solution $p(x, t)$ (2.43) (Right)

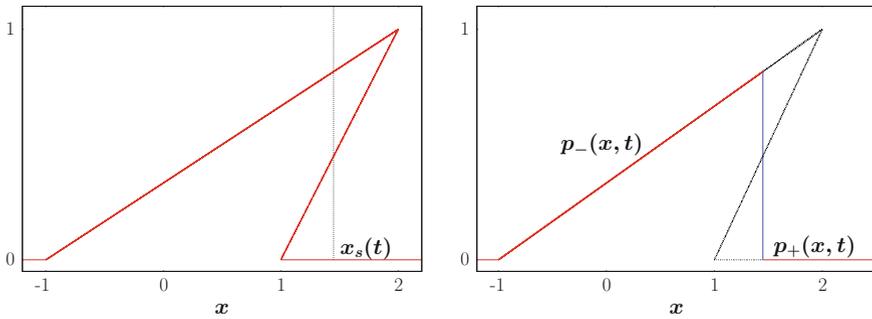


Fig. 2.4 (Left) The multivalued solution (2.43) and insertion of a shock at $x = x_s(t)$, (Right) reduction to a single-valued solution given by (2.46)

There is a systematic and rigorous approach for correcting this unphysical behaviour and modifying the solution to make it single-valued through the use of *shocks*. Shocks are moving jump discontinuities in the solution that separate one piecewise-defined portion of the solution ahead of the shock, $p_+(x, t)$, from another part behind the shock, $p_-(x, t)$, eliminating the multi-valued behaviour (see Fig. 2.4). Shock waves are common in many physical systems, including acoustics (sonic booms), fluid flow (hydraulic jumps), and traffic flow (moving traffic jams).

The construction of shock-corrected solutions builds on the idea that if a shock is inserted at one position, $x = x_s(t)$, it can appropriately separate the overlapping sets of characteristic curves to produce a well-defined single-valued solution everywhere away from the shock. The constructed solution should satisfy all of the properties expected for the conservation law and we use this to derive the equation for the motion of the shock position.

Consider a general quasilinear equation describing the transport of a property $p(x, t)$ according to a flux function $q = q(p)$,

$$\frac{\partial p}{\partial t} + \frac{\partial q(p)}{\partial x} = 0, \quad (2.44)$$

which has been derived for smooth solutions via the Reynolds transport theorem from a conservation law for p . The integrated form of (2.44) on a fixed domain $a \leq x \leq b$ includes contributions from fluxes at the ends of the domain,

$$\frac{d}{dt} \left(\int_a^b p \, dx \right) + q(p) \Big|_{x=a}^{x=b} = 0. \quad (2.45)$$

If a shock were inserted at some position $x = x_s(t)$, the piecewise-defined form of the solution becomes

$$p(x, t) = \begin{cases} p_-(x, t) & a \leq x < x_s(t), \\ p_+(x, t) & x_s(t) < x \leq b. \end{cases} \quad (2.46)$$

Separating (2.45) with respect to dependence on the solution to the left or right of the shock then yields

$$\left[\frac{d}{dt} \left(\int_a^{x_s} p_- dx \right) - q(p_-(a, t)) \right] + \left[\frac{d}{dt} \left(\int_{x_s}^b p_+ dx \right) + q(p_+(b, t)) \right] = 0. \quad (2.47)$$

Applying Leibniz's rule (2.8) then gives

$$\begin{aligned} \left(\int_a^{x_s} \frac{\partial p_-}{\partial t} dx + p_-(x_s, t) \frac{dx_s}{dt} \right) + \left(\int_{x_s}^b \frac{\partial p_+}{\partial t} dx - p_+(x_s, t) \frac{dx_s}{dt} \right) \\ + [q(p_+(b, t)) - q(p_-(a, t))] = 0. \end{aligned}$$

By adding and subtracting $q(p_{\pm})(x_s)$ and re-grouping terms, we obtain

$$\begin{aligned} \left(\int_a^{x_s} \partial_t p_- dx + q(p_-(x_s, t)) - q(p_-(a, t)) \right) \\ + \left(\int_{x_s}^b \partial_t p_+ dx + q(p_+(b, t)) - q(p_+(x_s, t)) \right) \\ - q(p_-(x_s, t)) + q(p_+(x_s, t)) + [p_-(x_s, t) - p_+(x_s, t)] \frac{dx_s}{dt} = 0. \end{aligned}$$

The terms in parentheses on the first two lines vanish based on applying (2.45) to the smooth solutions on the sub-intervals $a \leq x < x_s$ and $x_s < x \leq b$ respectively. The remaining terms give the so-called *Rankine–Hugoniot shock speed relation*

$$\frac{dx_s}{dt} = \frac{q(p_+(x_s, t)) - q(p_-(x_s, t))}{p_+(x_s, t) - p_-(x_s, t)}. \quad (2.48)$$

For the inviscid Burgers equation (2.39), the flux is $q(p) = \frac{1}{2}p^2$, and for our specific example, $p_-(x, t) = (1+x)/(1+t)$ and $p_+(x, t) = 0$ yielding the shock speed equation,

$$\frac{dx_s}{dt} = \frac{p_+(x_s, t) - p_-(x_s, t)}{2} \implies \frac{dx_s}{dt} = \frac{1 + x_s}{2(1+t)}. \quad (2.49)$$

Initial conditions for this equation are determined by the time and position where characteristics first cross, necessitating the insertion of a shock; in this case, $x_s(1) = 1$. Consequently the position of the shock is given by

$$x_s(t) = \sqrt{2(1+t)} - 1 \quad \text{for } t \geq 1.$$

Fig. 2.5 Characteristic curves in the xt plane truncated by the shock $x = x_s(t)$ corresponding to (2.46)

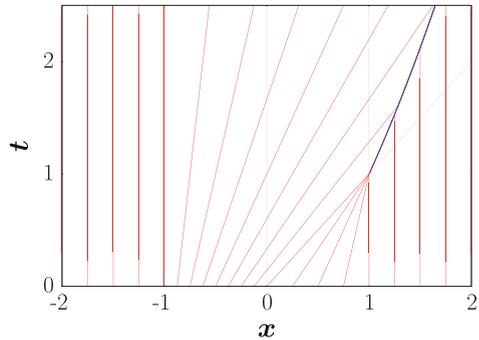


Figure 2.5 shows the shock in the xt plane in its role in separating families of characteristics that would otherwise intersect. Excluding the shock curve, Fig. 2.5 has a single characteristic curve passing through each (x, t) point and hence describes a single-valued solution of the transport problem. This figure differs from Fig. 2.4 (left) only in the wedge-shaped region bounded by the curves $x = 1$ and $x = t$ that form the boundaries of what is sometimes called the *shock envelope*.

Returning to Fig. 2.3, we note that our solution $p(x, t)$ began as an equilateral triangle on $-1 \leq x \leq 1$ with height one, and hence area one. As time increases the profile steepens toward the right while maintaining its base and height, and hence area, even as it transitions from being an acute triangle (single-valued solution) to an obtuse triangle (multivalued solution) (also see Fig. 2.4 (left)). The consequence of introducing the shock is to cut out the portion of (2.43) that overturns while modifying the domains on which the other parts of the solution apply for $t \geq 1$,

$$p(x, t) = \begin{cases} 0 & x < -1, \\ (1+x)/(1+t) & -1 \leq x \leq x_s(t), \\ 0 & x > x_s(t). \end{cases} \quad (2.50)$$

The resulting solution profiles are right triangles on the base $-1 \leq x \leq x_s(t)$ and p ranging over $0 \leq p \leq \max p = p_-(x_s(t), t) = \sqrt{2}/(1+t)$. To satisfy the conservation of the integral of p , (2.48) ensures that the shock maintains the area of $A = \frac{1}{2}(\text{base})(\text{height}) = \frac{1}{2}(\sqrt{2(1+t)} - 1 - (-1))(1/\sqrt{2(1+t)}) = 1$. This illustrates why the shock selection rule is sometimes called the *equal-area rule*.² Later, we will see in Chap. 5 that solution (2.50) can also be obtained as a *similarity solution*.

²See Fig. 2.4—the placement of the shock not only conserves the area of the newly-formed right triangle, but also requires that the areas of the two cut-off multi-valued regions from the obtuse triangle to be equal.

2.7 Further Directions

The classic text on linear and nonlinear waves is the book by Whitham [106]. There are additional more recent books on waves [65, 80] and the method of characteristics and its extensions are covered in detail in most books on applied partial differential equations and modelling (see [45, 81], for example).

2.8 Exercises

2.1 Let $x = a(t)$ and $x = b(t)$ be positions of two points that move according to a flow $dx/dt = v(x, t)$, then if

$$f_{\text{avg}}(t) = \frac{1}{b(t) - a(t)} \int_{a(t)}^{b(t)} f(x, t) dx,$$

calculate $\lim_{b \rightarrow a} \frac{df_{\text{avg}}}{dt}$. Hint: Let $b(t) = a(t) + \varepsilon h(t)$ with $\varepsilon \rightarrow 0$.

2.2 In one dimension, the *Euler equations* for compressible gas dynamics are

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho v) = 0, \quad \rho \left(\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} \right) = -\frac{\partial P}{\partial x},$$

where the gradient of the pressure $P(x, t)$ represents an internal force generated by the gas. Note that the left-hand side of the second equation can be written in terms of the convective derivative, $\rho Dv/Dt$. The first equation is the continuity equation for the conservation of mass. Show that the second equation is consistent with the conservation of momentum with non-constant density,

$$\frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho v^2)}{\partial x} = -\frac{\partial P}{\partial x}.$$

2.3 Consider the solution of a linear wave equation having the dispersion relation $\omega = \omega(k)$,

$$\rho(x, t) = \cos(kx - \omega(k)t) + \cos([k + \varepsilon]x - \omega(k + \varepsilon)t).$$

(a) Show that for $\varepsilon \rightarrow 0$ this can be re-written in terms of the *phase velocity*, c_p , and *group velocity*, c_g , as

$$\rho(x, t) = 2 \cos(k[x - c_p(k)t]) \cos\left(\frac{1}{2}\varepsilon[x - c_g(k)t]\right) + O(\varepsilon)$$

What is the formula for the group velocity for $\varepsilon \rightarrow 0$?

(b) Use $\rho(x, t) = \cos(kx - \omega t)$ to determine the dispersion relation for the equation

$$\rho_t + \rho_x - \rho_{xxt} = 0 \quad (2.51)$$

and calculate the group velocity. Also determine the “modified dispersion relation” $\tilde{\omega}(k)$ from $\rho(x, t) = e^{kx - \tilde{\omega}t}$, which will be used in the next exercise.

2.4 Solitons (or “solitary waves”) are steady profile travelling waves describing a single “pulse” whose size and speed are connected through nonlinear effects. Consider the nonlinear wave equation,

$$\rho_t + \rho_x + 6\rho\rho_x - \rho_{xxt} = 0,$$

called the *Benjamin-Bona-Mahony equation*.

- (a) By looking for solutions of the PDE in travelling wave form, $\rho(x, t) = P(x - ct)$, determine the ODE for $P(s)$ with $s = x - ct$.
 (b) Show that there is a one-parameter family of solutions of the form

$$P(s) = A \operatorname{sech}^2(Bs)$$

and determine how A and B are related to the speed c .

- (c) Show that the nonlinear solitary wave surprisingly satisfies the modified dispersion relation from the linearised equation (2.51).

2.5 Dispersion relations are not limited to being algebraic relations. Consider the following fluid dynamics model of water waves, given in terms of a potential function $\phi(x, y, t)$ (defined on $0 \leq y \leq 1$) and a wave profile $f(x, t)$ on the surface of the water (at $y = 0$),

$$\begin{aligned} \phi_{xx} + \phi_{yy} &= 0 & \text{on } 0 \leq y \leq 1, \\ \phi_y &= 0 & \text{at } y = 0, \\ \phi_t + f &= 0 & \text{at } y = 1, \\ f_t &= \phi_y & \text{at } y = 1. \end{aligned}$$

Assume the wave is $f(x, t) = A \cos(kx - \omega t)$. Show that the corresponding potential must be of the form $\phi(x, y, t) = B(y) \sin(kx - \omega t)$ and obtain the dispersion relation $\omega(k)$.

2.6 Obtain explicit solutions $\rho = \rho(x, t)$ for $t \geq 0$ for the following problems,

- (a) The initial value problem for $\rho(x, t)$ on $-\infty < x < \infty$:

$$\frac{\partial \rho}{\partial t} + e^{2t} \frac{\partial \rho}{\partial x} = \rho + x + t, \quad \rho(x, t = 0) = \cos x.$$

(b) The signalling problem³ for $\rho(x, t)$ on $x \geq 0$:

$$\frac{\partial \rho}{\partial t} + (x + 4) \frac{\partial \rho}{\partial x} = -2\rho, \quad \rho(x = 0, t) = \cos t, \quad \rho(x, t = 0) = e^{-x}.$$

2.7 A one-dimensional compressible fluid blob starts at $t = 0$ with uniform density $\rho \equiv 1$ on $1 \leq x \leq 2$. The blob obeys the conservation of mass equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho v)}{\partial x} = 0.$$

with the (Eulerian) velocity field given as $v(x, t) = x^2 e^{-3t}$.

- (a) Find the density of the blob for $t \geq 0$ as a function of position and time, $\rho = \rho(x, t)$.
- (b) Find the positions of the moving left and right edges of the blob, $x_1(t) \leq x \leq x_2(t)$.
- (c) Use your results from parts (a, b) to directly evaluate the integral

$$\int_{x_1(t)}^{x_2(t)} \rho(x, t) dx$$

and show that this is consistent with the Reynolds transport theorem.

2.8 (*The method of characteristics in two dimensions*) At time $t = 0$, a radioactive substance is released into a steady two-dimensional flow. The initial concentration of the substance is given by

$$c_0(x, y) = \begin{cases} 1 - (x^2 + y^2) & x^2 + y^2 \leq 1, \\ 0 & \text{else.} \end{cases}$$

In the absence of flow, the concentration would decay according to the rate equation $dc/dt = -c$. The substance is carried by the two-dimensional Eulerian velocity field $\mathbf{v} = (1 + x, y)$.

(a) The conservation law for the decaying substance on any fluid blob $D(t)$ is

$$\frac{d}{dt} \left(\iint_{D(t)} c dA \right) = - \iint_{D(t)} c dA.$$

Use the Reynolds transport theorem to derive the PDE for the concentration field $c(x, y, t)$.

(b) Instead of writing “ $\mathbf{A} = (x_0, y_0)$ ” as a material coordinate in rectangular coordinates, parametrise the initial data in terms of polar material coordinates (R, Θ) .

³A wave being specified by a boundary condition from a fixed “signal source” position.

Write the characteristic ODEs (dX/dt , dY/dt , dC/dt) and solve these equations with the given initial conditions.

- (c) Obtain the explicit Eulerian solution $c(x, y, t)$.
- (d) The boundary of the region over which the substance has spread remains circular for all times; find its radius and the coordinates of its centre as functions of time.

2.9 Consider the system of wave equations

$$\begin{aligned} p_t + 5p_x - 7q_x &= 0, \\ q_t + 2p_x - 4q_x &= 0. \end{aligned}$$

- (a) Find the eigenvalues and eigenvectors for travelling waves in this system.
- (b) Find the solutions $p(x, t)$ and $q(x, t)$ if the initial conditions at $t = 0$ are

$$p(x, 0) = 5 \sin(7x), \quad q(x, 0) = -9 \cos(4x).$$

2.10 The classic wave equation is

$$\frac{\partial^2 \phi}{\partial t^2} = c^2 \frac{\partial^2 \phi}{\partial x^2}. \tag{2.52}$$

It can be used to describe small transverse vibrations of a displaced string (like a guitar or violin string) starting from initial conditions for the position and velocity of each point along the string at $t = 0$:

$$\phi(x, 0) = f(x), \quad \phi_t(x, 0) = g(x).$$

- (a) Show that this problem can be written as a system of first order wave equations:

$$p_t - c^2 q_x = 0, \quad q_t - p_x = 0,$$

where $q = \phi_x$ and $p = \phi_t$.

- (b) Solve the system to obtain $p(x, t)$ and $q(x, t)$ in terms of travelling waves.
- (c) Show that from (b) we can write the solution of the original problem as

$$\phi(x, t) = A(x - ct) + B(x + ct).$$

- (d) Determine the functions $A(x)$ and $B(x)$ in terms of the initial data, functions $f(x)$ and $g(x)$. This form of the solution is called the *D'Alembert solution*.

2.11 The shallow water equations describe fluid flow in shallow (long, slender) layers, such as rivers. In simplest form, they are

$$\frac{\partial h}{\partial t} + h \frac{\partial v}{\partial x} + v \frac{\partial h}{\partial x} = 0, \quad \frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} + g \frac{\partial h}{\partial x} = 0,$$

where $v(x, t)$ is the fluid speed, $h(x, t)$ is the height of the fluid layer, and g is the acceleration due to gravity.

Show that the shallow water equations correspond to the following Lagrangian statements about conservation of mass and change of momentum for all fluid blobs moving with the flow:

$$\frac{d}{dt} \left(\int_{a(t)}^{b(t)} h \, dx \right) = 0, \quad \frac{d}{dt} \left(\int_{a(t)}^{b(t)} hv \, dx \right) = -G(h) \Big|_{x=a}^{x=b}$$

Determine the function $G(h)$.

2.12 To completely specify the problem for the determination of the position of a shock in the Rankine–Hugoniot equation (2.48), we must provide initial conditions on when/where the shock first forms, $x_s(t_*) = x_*$.

Consider the transport equation $p_t + q(p)_x = 0$ with initial condition $p(x, 0) = f(x)$. Assume that $q'(p) > 0$ and $f(x)$ has a local maximum (for example, $f(x) = e^{-x^2}$).

- Consider two characteristic curves, $x = X(t; A_0)$ and $x = X(t; A_1)$, and assume that they carry different values of the solution ($P_0 \neq P_1$). Determine the position, $x_{0,1}$, and time, $t_{0,1}$, where they will intersect.
- Determine the time when the shock first forms, t_* in terms of q, f , by minimising the (positive) intersection time over all pairs of characteristics. Hint: Consider the limit of two characteristics starting very close together.

2.13 (*Shocks in quasilinear equations*) Consider the inviscid Burgers equation,

$$\frac{\partial p}{\partial t} + p \frac{\partial p}{\partial x} = 0,$$

starting from the initial conditions

$$p(x, t = 0) = \begin{cases} 9 - x^2 & |x| \leq 3, \\ 0 & |x| > 3. \end{cases}$$

- Use the method of characteristics to construct the parametric solution.
- Eliminate the parameter from the solution found in part (a) to obtain a multi-valued solution in two parts.
- Determine the time t_* and x_* -position where $x(t)$ characteristic curves first intersect (see Exercise 2.12).

- (d) Use the results from parts (b, c) along with the shock speed equation (2.48) to write the ODE initial value problem for the shock position $x_s(t)$.
- (e) Write the inviscid Burgers equation as a conservation law, state the conserved quantity (with the specific value set by the above initial condition), and integrate using the solution from (b) to produce an algebraic equation involving t and $x_s(t)$.

2.14 Consider the (viscous) Burgers equation

$$\frac{\partial p}{\partial t} + p \frac{\partial p}{\partial x} = \varepsilon^2 \frac{\partial^2 p}{\partial x^2} \quad \varepsilon \rightarrow 0$$

subject to boundary conditions

$$p(x \rightarrow -\infty) = 2, \quad p(x \rightarrow \infty) = 1.$$

Determine the first order ODE satisfied by travelling wave solutions, $p(x, t) = P(x - ct)$. Solve the ODE and apply the boundary conditions to determine travelling wave profile $P(s)$ and the wave speed c . Show that this matches the shock speed that would be obtained with $\varepsilon = 0$, for (2.39).

2.15 (*Fully-nonlinear first order PDEs*) The most general first-order PDE involving only first derivatives of a solution $p(x, t)$ can be written as

$$F(p, p_x, p_t, x, t) = 0,$$

where F is a given function. Let s be a parametric variable and parametrise all quantities in terms of s as

$$x = X(s) \quad t = T(s) \quad p = P(s) \quad p_x = R(s) \quad p_t = Q(s)$$

- (a) Starting from $P(s) = p(X(s), T(s))$ take the derivative of P with respect to s and use the chain rule to express dP/ds in terms of R, Q, X', T' .
- (b) Take the s -derivative of $F = 0$ using the chain rule and then use the result from part (a) to write the equation in the form

$$\frac{dF}{ds} = \underbrace{\left[A \frac{dR}{ds} + B \frac{dX}{ds} \right]}_{=0} + \underbrace{\left[C \frac{dQ}{ds} + D \frac{dT}{ds} \right]}_{=0} = 0.$$

Note that selecting $X' = A, R' = -B, T' = C, Q' = -D$ satisfies the overall equation.

Obtain a system of five autonomous ODEs for X, T, P, R, Q in terms of those variables and derivatives of F .

- (c) Determine the characteristic equations for the general *Hamilton–Jacobi PDE*,

$$p_t + H(p, p_x, x, t) = 0,$$

where H is a given function.

- (d) Obtain the parametric solution, $X(A, t), P(A, t)$ for the problem for $p(x, t)$ on $-\infty < x < \infty$ and $t \geq 0$,

$$\frac{\partial p}{\partial t} + \left(\frac{\partial p}{\partial x} \right)^4 = 0, \quad p(x, 0) = e^{-x^2}.$$