15

Splitting Schemes for PDEs with Source Terms

15.1 Introduction

This chapter is concerned with numerical methods for solving non–linear systems of hyperbolic conservation laws with source terms

$$\mathbf{U}_t + \mathbf{F}(\mathbf{U})_x = \mathbf{S}(\mathbf{U}) \; . \tag{15.1}$$

$\mathbf{U}$ is the vector of unknowns, $\mathbf{F}(\mathbf{U})$ is the vector of fluxes and $\mathbf{S}(\mathbf{U})$ is a vector of *sources*, which in general is an algebraic function of $\mathbf{U}$ or other physical parameters of the problem at hand. In Chap. 2 we studied some properties for the *pure advection* hyperbolic problem

$$\mathbf{U}_t + \mathbf{F}(\mathbf{U})_x = \mathbf{0} \; . \tag{15.2}$$

This *homogeneous system*, in which $\mathbf{S}(\mathbf{U}) \equiv \mathbf{0}$ (no sources) is a simplified version of (15.1). The time–dependent one dimensional Euler equations of Chap. 3 are one example of a homogeneous system of this kind. Another simplification of (15.1) results from the assumption of no spatial variations, $\mathbf{F}(\mathbf{U})_x = \mathbf{0}$, in which case one obtains

$$\frac{d}{dt}\mathbf{U} = \mathbf{S}(\mathbf{U}) \; , \tag{15.3}$$

which is a system of Ordinary Differential Equations (ODEs).

Inhomogeneous systems of the form (15.1), $\mathbf{S}(\mathbf{U}) \neq \mathbf{0}$, arise naturally in many problems of practical interest. A whole class of inhomogeneous systems are derived when reducing the spatial dimensionality of multidimensional problems. For example, under the assumption of spherically or cylindrically symmetric flow, the three or two dimensional Euler equations become a one–dimensional system of the form (15.1); see Sect. 1.6.2 of Chap. 1. In this case the source terms are geometric in character. Sources of similar type are present in the shallow water equations for flow on non–horizontal channels; see Sect. 1.6.3 of Chap. 1.

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Important examples of inhomogeneous systems of the form (15.1) arise in the study of the fluid dynamics of reactive gaseous mixtures, where in addition to the fluid dynamics governed by a system like (15.2), there are chemical reactions between the constituent gases, which in the absence of fluid flow may be modelled by systems of the form (15.3). Examples of problems of this kind arise in the study of hypersonic flows [119], [9] and detonation waves, see for instance [191], [72], [78], [118] and [363].

Chemically active flows contain a range of widely varying time scales, which leads to *stiff* ODEs of the form (15.3), [296]. The problem of *stiffness* in ODEs may be resolved by resorting to *implicit methods*. For chemically active flow models (15.1), stiffness may not be resolved by simply using implicit methods. If the mesh is not sufficiently fine in both space and time, then spurious solutions travelling at unphysical speeds may be computed [136], [314], [49], [78], [227]. See also the recent review paper by Yee and Sweby [594]. There are still a number of unresolved problems in solving systems like (15.2), which are the subject of current research.

There are essentially two ways of constructing methods to solve inhomogeneous systems of the form (15.1). One approach attempts to preserve some coupling between the two processes in (15.1). These two processes might be represented by the systems (15.2) (advection) and (15.3) (reaction–like). LeVeque and Yee [314] report on a predictor–corrector scheme of the MacCormack type with a TVD constraint. The idea of *upwinding the source terms* [412], may be seen as an attempt to couple the two processes involved, although the eigenstructure used in projecting the source terms is oblivious to the influence of these.

Another approach is to *split* (15.1), for a time Δt, into the advection problem (15.2) and the source problem (15.3). At first sight this might appear unreasonable. However, for the case of a model inhomogeneous PDE, splitting is actually exact. For more general problems, the fact that one can construct high–order splitting schemes following this approach is also somewhat reassuring. In addition, computational experience suggests that splitting is a viable approach, *if used with caution*. The main attraction of splitting schemes is in the fact that one can deploy the optimal, existing schemes for each subproblem. For instance, to solve the homogeneous subproblem (15.2) one may use directly any of the schemes presented in Chaps. 6 to 14, or any other appropriate method. To solve the subproblem (15.3) one may use directly any of the ODE solvers available. If the system is known to be stiff, then *stiff* solvers must be used.

This chapter is concerned with splitting schemes to solve (15.1). In Sect. 15.2 we show that for a model equation, splitting is exact; in Sect. 15.3 we present numerical schemes based on the splitting approach; in Sect. 15.4 we briefly review some basic aspects of numerical methods for Ordinary Differential Equations (ODEs). Concluding remarks are given in Sect. 15.5.

15.2 Splitting for a Model Equation

The simplest model hyperbolic equation of the form (15.1) is given by

$$u_t + au_x = \lambda u \ , \tag{15.4}$$

where a is constant wave propagation speed and λ is a constant parameter. This simple model equation will prove very useful in discussing possible strategies for solving (15.1) numerically.

Consider the initial value problem (IVP) for (15.4), namely

$$\left.\begin{array}{l} \text{PDE} : u_t + au_x = \lambda u \ , \\ \text{IC} \quad : u(x,0) = u_0(x) \ . \end{array}\right\} \tag{15.5}$$

Here $u = u(x,t)$, $-\infty < x < \infty$, $t > 0$ and $u_0(x)$ is the initial data for the problem at $t = 0$. It is easy to verify that the exact solution of IVP (15.5) is

$$u(x,t) = u_0(x - at)e^{\lambda t} \ . \tag{15.6}$$

Note in particular that if $\lambda = 0$ we recover the exact solution for the homogeneous equation $u_t + au_x = 0$, namely $u_0(x - at)$; see Sect. 2.2 of Chap. 2.

A geometric interpretation of the original IVP (15.5) results if we view (15.5) as an IVP involving an ODE along characteristics, namely

$$\left.\begin{array}{l} \frac{d}{dt}u = \lambda u \ ; u(0) = u(x_0) \ , \\ \frac{d}{dt}x = a \quad ; x(0) = x_0 \ . \end{array}\right\} \tag{15.7}$$

Fig. 15. 1 illustrates the situation. The ODE in (15.7) requires initial data at

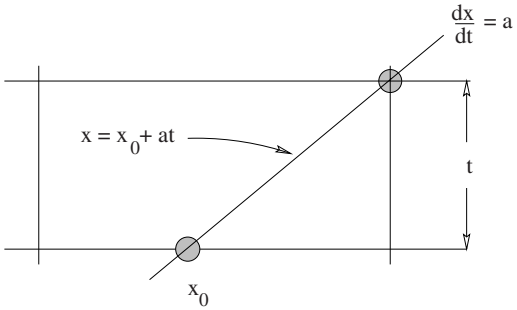

Fig. 15.1. Illustration of operator splitting scheme for model PDE with source term

the foot of the characteristic curve $x = x_0 + at$, namely the point x_0. Actually the initial data is then $u(0) = u(x_0) = u(x - at)$, which is the solution of the homogeneous problem in (15.5), $\lambda = 0$.

Next we show that the exact solution (15.6) can also be obtained by solving exactly a pair of initial value problems in succession.

Theorem 15.1 (Splitting of Source Term).
The exact solution (15.6) of the inhomogeneous IVP (15.5) can be found by solving exactly the following pair of IVP's.

$$\left.\begin{array}{l} PDE: r_t + a r_x = 0 \ , \\ IC \quad : r(x,0) = u_0(x) \ , \end{array}\right\} \Longrightarrow r(x,t) \tag{15.8}$$

$$\left.\begin{array}{l} ODE: \frac{d}{dt} s = \lambda s \ , \\ IC \quad : s(0) = r(x,t) \ , \end{array}\right\} \Longrightarrow u(x,t) \tag{15.9}$$

Note here that the initial condition of IVP (15.8) is the actual initial condition for the original IVP (15.5) and the initial condition for IVP (15.9) is the solution $r(x,t)$ of IVP (15.8).

Proof. Clearly the solution of IVP (15.8) is $r(x,t) = u_0(x-at)$, while the exact solution of IVP (15.9) is $s(x(t),t) = s(0)e^{\lambda t}$. But $s(0) = r(x,t) = u_0(x-at)$ and thus the resulting solution of IVPs (15.8) and (15.9) is

$$s(x,t) = u_0(x-at)e^{\lambda t} \ ,$$

which is the exact solution (15.6) of the original inhomogeneous IVP (15.5), and the theorem is thus proved.

The result on the splitting scheme obtained by solving in succession (15.8), (15.9) can be expressed in the succinct form

$$u(x,t) = S^{(t)} C^{(t)} [u_0(x)] \ . \tag{15.10}$$

We interpret $C^{(t)}$ as the *solution operator* for the advection problem (15.8) applied over a time t and $S^{(t)}$ as the *solution operator* for the ODE (15.9) applied for a time t.

Exercise 15.2. Show that the exact solution $u(x,t)$ of IVP (15.5) can be obtained by solving

$$\left.\begin{array}{l} \text{PDE} : u_t + f(u)_x = 0 \ ; f(u) = au \ , \\ \text{IC} \quad : u(x,0) = u_0(x) \end{array}\right\} \Longrightarrow \overline{u}^{n+1} \tag{15.11}$$

and

$$\left.\begin{array}{l} \text{ODE} : \frac{d}{dx} f(u) = \lambda u \ , \\ \text{IC} \quad : \overline{u}^{n+1} \end{array}\right\} \Longrightarrow u^{n+1} \tag{15.12}$$

in succession.

This result says that the splitting scheme (15.8), (15.9) modified by replacing the ODE in time by an ODE in space also gives the exact solution. This splitting scheme can be expressed in the succinct form

$$u(x,t) = S^{(x)} C^{(t)} [u_0(x)] \ , \tag{15.13}$$

where $S^{(x)}$ denotes the solution operator for the ODE in x in (15.12).

Solution 15.3. Left to the reader.

Glimm, Marshall and Plohr [214] constructed numerical splitting schemes of the form (15.11), (15.12) to solve numerically one–dimensional flows with area variation. In this case the source term involves a spatial derivative and does not depend on time.

In the next section we construct numerical methods based on the splitting approach, or fractional step approach [466], [588].

15.3 Numerical Methods Based on Splitting

We have shown that for the model inhomogeneous PDE (15.4) the splitting approach, as described in the previous section, is *exact*. For non–linear systems (15.1) this result is no longer valid. However, approximate, numerical schemes based on the splitting approach can be constructed. We first consider the scalar case.

15.3.1 Model Equations

The splitting scheme (15.8)–(15.9), represented by (15.10), is exact if the operators C and S are exact. Here we are interested in constructing numerical methods for the scalar IVP

$$\left.\begin{array}{l} \text{PDE} : u_t + f(u)_x = s(u) : \ 0 \leq x \leq L \ , \\ \text{IC} \quad : u(x, t^n) = u^n \ , \end{array}\right\} \tag{15.14}$$

To this end we replace the exact operators $C^{(t)}$ and $S^{(t)}$ in (15.10) by approximate operators and re–state the problem in a numerical context. Given the IVP (15.14), we want to evolve the solution from its initial value u^n at a time t^n, by one time step of size Δt, to a value u^{n+1} at time $t^{n+1} = t^n + \Delta t$. We assume the spatial domain $[0, L]$ has been discretised into a finite number M of cells i (finite volume approach) or grid points i (finite difference approach). Here u^n is a set of discrete values u_i^n at time t^n. The discrete analogue of the splitting scheme (15.8)–(15.9) is now

$$\left.\begin{array}{l} \text{PDE} : u_t + f(u)_x = 0 \ , \\ \text{IC} \quad : u(x, t^n) = u^n \ , \end{array}\right\} \Longrightarrow \overline{u}^{n+1} \tag{15.15}$$

$$\left.\begin{array}{l} \text{ODE} : \frac{d}{dt} u = s(u) \ , \\ \text{IC} \quad : \overline{u}^{n+1} \ . \end{array}\right\} \Longrightarrow u^{n+1} \tag{15.16}$$

The initial condition for the advection problem (15.15) is the initial condition for the complete problem (15.14). The solution of (15.15) after a time Δt is denoted by $\overline{u}^{n+1}$ and is used as the initial condition for the second IVP (15.16). This second IVP accounts for the presence of the source term $s(u)$

and is also solved for a complete time step Δt; this solution is then regarded as an approximation to the solution u^{n+1} of the full problem (15.14) at a time $t^{n+1} = t^n + \Delta t$. If the numerical analogues of $S^{(t)}$ and $C^{(t)}$ in (15.10) are still denoted by S and C, then we can write the splitting of (15.14) into (15.15)–(15.16) as

$$u^{n+1} = S^{(\Delta t)} C^{(\Delta t)}(u^n) \; . \tag{15.17}$$

Each numerical sub–problem (15.15), (15.16) is dealt with separately, for a time step Δt. One requires a numerical method to solve the homogeneous advection problem (15.15) and another numerical method to solve the ordinary differential equation in (15.16), with the initial data taken from the solution of (15.15). This procedure for solving inhomogeneous systems is exceedingly simple but is only first–order accurate in time, when S and C are at least first–order accurate solution operators. A second–order accurate scheme is

$$u^{n+1} = S^{(\frac{1}{2}\Delta t)} C^{(\Delta t)} S^{(\frac{1}{2}\Delta t)}(u^n) \; , \tag{15.18}$$

where S and C are at least second–order accurate solution operators.

15.3.2 Schemes for Systems

Here we extend the application of the splitting scheme of the previous section to non–linear systems of the form (15.1). The generalisation of (15.15), (15.16) to solve (15.1) is straightforward. Given the IVP

$$\left.\begin{array}{l} \text{PDE's} : \mathbf{U}_t + \mathbf{F}(\mathbf{U})_x = \mathbf{S}(\mathbf{U}) \; ; 0 \le x \le L \; , \\ \text{IC} \quad\; : \mathbf{U}(x, t^n) = \mathbf{U}^n \; , \end{array}\right\} \tag{15.19}$$

we want to evolve $\mathbf{U}^n$ from time $t = t^n$ to the new value $\mathbf{U}^{n+1}$ at $t = t^{n+1}$ in a time step $\Delta t = t^{n+1} - t^n$. The splitting (15.15), (15.16) becomes

$$\left.\begin{array}{l} \text{PDE's} : \mathbf{U}_t + \mathbf{F}(\mathbf{U})_x = \mathbf{0} \; , \\ \text{IC} \quad\; : \mathbf{U}(x, t^n) = \mathbf{U}^n \end{array}\right\} \Longrightarrow \overline{\mathbf{U}}^{n+1} \; , \tag{15.20}$$

$$\left.\begin{array}{l} \text{PDE's} : \frac{d}{dt}\mathbf{U} = \mathbf{S}(\mathbf{U}) \; , \\ \text{IC's} \quad\; : \overline{\mathbf{U}}^{n+1} \end{array}\right\} \Longrightarrow \mathbf{U}^{n+1} \; . \tag{15.21}$$

The analogue of the first–order scheme (15.17) is

$$\mathbf{U}^{n+1} = S^{(\Delta t)} C^{(\Delta t)}(\mathbf{U}^n) \; . \tag{15.22}$$

A second–order accurate scheme for systems is

$$\mathbf{U}^{n+1} = S^{(\frac{1}{2}\Delta t)} C^{(\Delta t)} S^{(\frac{1}{2}\Delta t)}(\mathbf{U}^n) \; . \tag{15.23}$$

A splitting scheme based on (15.11), (15.12) is

$$\left.\begin{array}{ll} \text{PDEs} : \mathbf{U}_t + \mathbf{F}(\mathbf{U})_x = \mathbf{0} \ , \\ \text{IC} \quad\ : \mathbf{U}(x, t^n) = \mathbf{U}^n \ , \end{array}\right\} \Longrightarrow \overline{\mathbf{U}}^{n+1} \tag{15.24}$$

$$\left.\begin{array}{ll} \text{ODEs} : \frac{d}{dx}\mathbf{F}(\mathbf{U}) = \mathbf{S}(\mathbf{U}) \ , \\ \text{IC} \quad\ : \overline{\mathbf{U}}^{n+1} \ . \end{array}\right\} \Longrightarrow \mathbf{U}^{n+1} \tag{15.25}$$

There appears to be little experience in using this approach. For source terms that are independent of time or involve spatial derivatives, this approach may be advantageous. See [214].

The attraction of splitting schemes is in the freedom available in choosing the numerical operators S and C. In general, one may choose the best scheme for each type of problems. For solving the advection (homogeneous) IVP (15.20) one can, for instance, use any of the schemes studied in Chaps. 6 to 14, or some other method. For solving the ODEs in (15.21), (15.25) one may choose some appropriate ODE solver, see next section.

15.4 Remarks on ODE Solvers

There is a vast literature on ODEs and on numerical methods for solving ODEs. For theoretical properties of ODEs see for example Brown [81], Ince and Sneddon [260], Sánchez [423] and Coddington and Levinson [130]. Almost any textbook on Numerical Analysis will contain some chapter on schemes for ODEs. See for example Hildebrand [249]; Mathews [347]; Conte and de Boor [139]; Maron and Lopez [337]; Johnson and Riess [273]; Kahaner, Moler and Nash [275]. Advanced textbooks are those of Gear [200], Lambert [296] and Shampine [441].

15.4.1 First–Order Systems of ODEs

Here we recall some very basic facts about first–order systems of ODEs

$$\frac{d}{dt}\mathbf{U}(t) \equiv \mathbf{U}' = \mathbf{S}(t, \mathbf{U}(t)) \ . \tag{15.26}$$

Here $\mathbf{U} = \mathbf{U}(t)$ and $\mathbf{S}(t, \mathbf{U}(t))$ are vector–valued functions of m components

$$\mathbf{U} = [u_1, u_2, \ldots, u_m]^T \ ; \quad \mathbf{S} = [s_1, s_2, \ldots, s_m]^T \tag{15.27}$$

and the independent variable t is a time–like variable. The Jacobian $\mathbf{A}(\mathbf{U})$ is defined as the matrix

$$\mathbf{A}(\mathbf{U}) = \partial\mathbf{S}/\partial\mathbf{U} = \begin{bmatrix} \partial s_1/\partial u_1 & \ldots & \partial s_1/\partial u_m \\ \partial s_2/\partial u_1 & \ldots & \partial s_2/\partial u_m \\ \vdots & \vdots & \vdots \\ \partial s_m/\partial u_1 & \ldots & \partial s_m/\partial u_m \end{bmatrix} \ . \tag{15.28}$$

The entries a_{ij} of $\mathbf{A}(\mathbf{U})$ are partial derivatives of the components s_i of the vector $\mathbf{S}$ with respect to the components u_j of the vector $\mathbf{U}$, that is $a_{ij} = \partial s_i/\partial u_j$. The eigenvalues λ_i of $\mathbf{A}$ are the solutions of the *characteristic polynomial*

$$|\mathbf{A} - \lambda\mathbf{I}| = \det(\mathbf{A} - \lambda\mathbf{I}) = 0\,, \tag{15.29}$$

where $\mathbf{I}$ is the identity matrix. Generally, the eigenvalues are complex numbers. Trivially, the eigenvalue of the model ODE

$$u'(t) = \lambda u(t) \tag{15.30}$$

is λ. The behaviour of a system of ODEs is, in the main, determined by the behaviour of its eigenvalues. For instance, the exact solution of (15.30) with initial condition $u(0) = 1$ is $u(t) = e^{\lambda t}$. For t close to 0 the solution varies rapidly if the eigenvalue is negative and large in absolute value. For t away from zero the solution is almost indistinguishable from 0.

An important property of ODEs is that of *stability*. Generally speaking stable solutions are bounded. Note that the solution of the linear ODE (15.30) is bounded only if $\lambda < 0$. Geometrically, a solution $\mathbf{U}(t)$ is stable if any other solution of the ODE whose initial condition is sufficiently close to that of $\mathbf{U}(t)$ remains in a *tube* enclosing $\mathbf{U}(t)$. If the diameter of the tube tends to 0 as t tends to ∞, the solution is said to be *asymptotically stable*. Stability of solutions $\mathbf{U}(t)$ is characterised in terms of the eigenvalues λ_j of the Jacobian matrix. In particular if the real part of every eigenvalue is negative the solution is asymptotically stable.

Another feature of ODEs is that of *stiffness*. Stiff ODEs are usually associated with processes operating on disparate time scales. Chemical kinetics is a classical source of stiff ODEs. The stiffness of a system is generally determined by the behaviour of the eigenvalues of the system. In addition, the time interval over which the solution is sought is also a consideration in determining the stiffness of the system. There will be intervals of *rapid variations* (transient) of the solution and intervals of *slow variation*. The single ODE (15.30) is stiff for $\lambda \ll 0$ and for time t in the vicinity of 0.

Following Lambert [296], a nonlinear system of the form (15.26) is said to be stiff if

- (i) $Re(\lambda_j) < 0\,,\ \ j = 1, 2, \ldots, m$ and
- (ii) $\lambda_{max} \equiv \max_j |Re(\lambda_j)| \gg \lambda_{min} \equiv \min_j |Re(\lambda_j)|$.

Here $Re(\lambda_j)$ denotes the real part of the complex number λ_j. The stiffness ratio is defined as $R_{stif} = \lambda_{max}/\lambda_{min}$. Modest values of R_{stif}, e.g. 20, are sufficient to cause serious numerical difficulties to explicit methods. In real applications R_{stif} may be as large as 10^6.

Before thinking of numerical methods to solve ODEs, a fundamental question is to investigate whether the ODEs are stiff or not; this will determine the appropriate numerical methods to be used for solving the equations. See Kahaner, Moler and Nash [275], Gear [200] and Lambert [296].

15.4.2 Numerical Methods

We are interested in solving the Initial Value Problem (IVP) for (15.26) with initial condition

$$\mathbf{U}(t^0) = \mathbf{U}_0. \tag{15.31}$$

Discretise the domain of integration $[t^0, t^f]$ through the partition $t^0 < t^1 < t^2 \ldots < t^n < t^{n+1} \ldots < t^f$. One way of constructing numerical methods to solve the IVP (15.26), (15.31) is by using Taylor series expansions. Another way is to integrate (15.26) between t^n and t^{n+1} to obtain

$$\mathbf{U}(t^{n+1}) = \mathbf{U}(t^n) + \int_{t^n}^{t^{n+1}} \mathbf{S}(t, \mathbf{U}(t))dt \; . \tag{15.32}$$

Various numerical methods are obtained depending on the way the integral is evaluated. The *Euler Method* results from evaluating the integral at the *old* time,

$$\mathbf{U}^{n+1} = \mathbf{U}^n + \Delta t \mathbf{S}(t^n, \mathbf{U}^n) \; . \tag{15.33}$$

where $\Delta t = t^{n+1} - t^n$ is the time step and $\mathbf{U}^n \approx \mathbf{U}(t^n)$. The Euler method is *explicit* and first–order accurate. The *Backward Euler Method*, also first order accurate but *implicit*, results from evaluating the integral at the *new* time t^{n+1}, namely

$$\mathbf{U}^{n+1} = \mathbf{U}^n + \Delta t \mathbf{S}(t^{n+1}, \mathbf{U}^{n+1}) \; . \tag{15.34}$$

A second–order implicit method results from a *trapezium rule* approximation to the integral, giving the *Trapezoidal Method*

$$\mathbf{U}^{n+1} = \mathbf{U}^n + \frac{1}{2}\Delta t[\mathbf{S}(t^n, \mathbf{U}^n) + \mathbf{S}(t^{n+1}, \mathbf{U}^{n+1})] \; . \tag{15.35}$$

A second–order, two stage *Runge–Kutta method* (explicit) is

$$\left.\begin{array}{ll} \mathbf{K}_1 & = \Delta t \mathbf{S}(t^n, \mathbf{U}^n) \; , \\ \mathbf{K}_2 & = \Delta t \mathbf{S}(t^n + \Delta t, \mathbf{U}^n + \mathbf{K}_1) \; , \\ \mathbf{U}^{n+1} & = \mathbf{U}^n + \frac{1}{2}[\mathbf{K}_1 + \mathbf{K}_2] \; . \end{array}\right\} \tag{15.36}$$

A fourth–order, four stage Runge–Kutta method (explicit) is

$$\left.\begin{array}{ll} \mathbf{K}_1 & = \Delta t \mathbf{S}(t^n, \mathbf{U}^n) \; , \\ \mathbf{K}_2 & = \Delta t \mathbf{S}(t^n + \frac{1}{2}\Delta t, \mathbf{U}^n + \frac{1}{2}\mathbf{K}_1) \; , \\ \mathbf{K}_3 & = \Delta t \mathbf{S}(t^n + \frac{1}{2}\Delta t, \mathbf{U}^n + \frac{1}{2}\mathbf{K}_2) \; , \\ \mathbf{K}_4 & = \Delta t \mathbf{S}(t^n + \Delta t, \mathbf{U}^n + \mathbf{K}_3) \; , \\ \mathbf{U}^{n+1} & = \mathbf{U}^n + \frac{1}{6}[\mathbf{K}_1 + 2\mathbf{K}_2 + 2\mathbf{K}_3 + \mathbf{K}_4] \; . \end{array}\right\} \tag{15.37}$$

Stability of numerical methods is a most important issue. To illustrate this point consider the model ODE (15.30) as solved by the explicit Euler method (15.33). The scheme reads

$$u^{n+1} = (1 + \Delta t\lambda)u^n \ . \tag{15.38}$$

Clearly, for stability one requires that the ODE itself be stable, $\lambda < 0$, and that the *amplification factor* satisfy $|1 + \lambda\Delta t| \leq 1$. Therefore the time step Δt must satisfy the stability restriction

$$\Delta t \leq \frac{2}{|\lambda|} \ . \tag{15.39}$$

For large $|\lambda|$ (stiff ODE) Δt can be extremely small, which means that the method becomes very inefficient or even useless in practice.

On the other hand, the Trapezoidal method (15.35), which is implicit, gives

$$u^{n+1} = \frac{(1 + \frac{1}{2}\Delta t\lambda)}{(1 - \frac{1}{2}\Delta t\lambda)}u^n \ . \tag{15.40}$$

This is stable for any Δt, provided $\lambda \leq 0$, that is whenever the ODE itself is stable.

Explicit methods are much simpler to use than implicit methods. The latter require the solution of non–linear algebraic equations at each time step and are therefore much more expensive. However, as illustrated, for stiff problems implicit methods are the only methods to use in any practical situation.

15.4.3 Implementation Details for Split Schemes

There are two facts that need to be emphasised when solving ODEs in the context of the splitting schemes described in Sect. 15.3. First, at every time t^n, at each mesh point i one has a system of ODEs to solve; second, the time evolution of the ODEs is generally short and is dictated by the time step in the overall splitting scheme. This second point is relevant when choosing ODE solvers.

Before selecting a method, an analysis of the ODEs must be performed. If the problem is non–stiff then a high–order explicit method is recommended. A stability analysis of the method must be carried out and enforced when selecting the size of the time step Δt. For simplicity, let us assume we want to implement the first–order splitting scheme (15.22). A practical problem is to determine the time step Δt. One first determines the time step Δt_c for the advection problem (15.20). If this problem is solved by some explicit method, e.g. Godunov's first order upwind method (see Chap. 6), then Δt_c is found from some stability constraint, i.e. the Courant condition, see Chap. 6. The solution of the advection problem is found at every mesh point i and this gives $\overline{\mathbf{U}}^{n+1}$, which is then used as the initial data for the ODE step (15.21). If the ODEs are solved by some implicit method, then there will be no stability restriction on the time step, and therefore one can advance the solution via the ODE solver by a time $\Delta t_s = \Delta t_c$, in *one go*. However, if an explicit method is used to solve the ODEs, then a stable time step Δt_s must first be found.

If $\Delta t_s \geq \Delta t_c$, then one may again advance the solution via the ODEs by a time Δt_c in *one go*. Hence the final solution at time t^{n+1} has been advanced by a time $\Delta t = \Delta t_c$. If $\Delta t_s < \Delta t_c$, then one possibility is to update via the ODEs in k steps of size $\Delta t_k = \Delta t_c/k$, where k is a positive integer such such Δt_k is a stable time step for the ODE solver. The previous observations apply directly when implementing the second–order splitting scheme (15.23). A useful reference is Chiang and Hoffmann [108].

15.5 Concluding Remarks

We have only presented one approach for treating source terms. There are other approaches, but at the present time there appears to be no clear, and sufficiently general, alternative to splitting. The idea of *upwinding* the source terms proposed by Roe [412] appears to work well for certain problems. See for instance the work of Vázquez [568] and that of Bermúdez and Vázquez [51]. See also the recent paper of Vázquez [569], which addresses the issue of geometric and friction source terms in shallow water models. For steady–state problems computed by time–marching schemes the reader should consult the recent paper by LeVeque [310].

The reader is strongly encouraged to utilise problems with exact solutions, whenever available, to carefully assess the numerical methods before applying them to *the real problem*. The simplest test problem is the IVP (15.5) with exact solution (15.6). More scalar test problems are found in [314], [136], [227]. A test problem with exact solution for a 2×2 non–linear system is the so called Fickett detonation analogue [191], see also example 2.4.3 of Sect. 2.4.2 in Chap. 2. This problem is exploited in [118] for testing numerical methods for detonation waves in high–energy solids. For the Euler equations, a test problem with exact solution is reported in [120]. Details of the solution are given in [115] and applications are also shown in [412] and [471].

For certain types of problems, such as detonation waves, there are serious difficulties in designing numerical methods to properly account for the fluid dynamics and the chemistry. For sufficiently fine meshes such difficulties may be overcome but at a cost that is impossible to meet with current computing resources, if realistic problems in multidimensions are to be solved. Since the early papers by Colella, Majda and Roytburd [136] and that of LeVeque and Yee [314], there has been a noticeable increase in the interest for hyperbolic systems with source terms, both numerically and theoretically. See, amongst others: Griffiths, Stuart and Yee [227]; Berkenbosch, Kaasschieter and Boonkkamp [49]; Bourlioux, Majda and Roytburd [78]; Fey, Jeltsch and Müller [190]; Chalabi [98], [99], [100], [101]; Benkhaldoun and Chalabi [44]; Pember [377], [378]; Schroll and Tveito [432]; Schroll and Winther [434]; Schroll, Tveito and Winther [433]; Corberán and Gascón [140]; Lorenz and Schroll [333]; Lafon and Yee [294], [295]; and especially the review paper of Yee and Sweby [594].

The splitting approach may also be applied to treat diffusion like terms [82], [529] in exactly the same manner as for algebraic source terms. The splitting approach also offers one way of solving multidimensional problems; this topic is dealt with in Chap. 16.