APPENDIX

Convection-Diffusion Equations: Vector-Valued Variables

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D.1 The Taylor-Galerkin method used for vector-valued variables

The only method which adapts itself easily to the treatment of vector variables is that of the Taylor-Galerkin procedure. Here we can repeat the steps of Section 2.7 but now addressed to the vector-valued equation with which we started Chapter 2 (Eq. 2.1), which we rewrite here for convenience. Accordingly,

$$\frac{\partial \mathbf{\Phi}}{\partial t} + \frac{\partial \mathbf{F}_i}{\partial x_i} + \frac{\partial \mathbf{G}_i}{\partial x_i} + \mathbf{Q} = \mathbf{0} \tag{D.1}$$

Noting that now $\mathbf{\Phi}$ has multiple components, expanding $\mathbf{\Phi}$ by a Taylor series in time we have [1,2]

$$\mathbf{\Phi}^{n+1} = \mathbf{\Phi}^n + \Delta t \left.\frac{\partial \mathbf{\Phi}}{\partial t}\right|_n + \left.\frac{\Delta t^2}{2}\frac{\partial^2 \mathbf{\Phi}}{\partial t^2}\right|_{n+\theta} \tag{D.2}$$

where θ is a number such that $0 \le \theta \le 1$.

From Eq. (D.1),

$$\left[\frac{\partial \mathbf{\Phi}}{\partial t}\right]_n = -\left[\frac{\partial \mathbf{F}_i}{\partial x_i} + \frac{\partial \mathbf{G}_i}{\partial x_i} + \mathbf{Q}\right]_n \tag{D.3a}$$

and differentiating

$$\left[\frac{\partial^2 \mathbf{\Phi}}{\partial t^2}\right]_{n+\theta} = -\frac{\partial}{\partial t}\left[\frac{\partial \mathbf{F}_i}{\partial x_i} + \frac{\partial \mathbf{G}_i}{\partial x_i} + \mathbf{Q}\right]_{n+\theta} \tag{D.3b}$$

In the above we can write

$$\frac{\partial}{\partial t}\left(\frac{\partial \mathbf{F}_i}{\partial x_i}\right) \equiv \frac{\partial}{\partial x_i}\left(\frac{\partial \mathbf{F}_i}{\partial \mathbf{\Phi}}\frac{\partial \mathbf{\Phi}}{\partial t}\right) = -\frac{\partial}{\partial x_i}\left[\mathbf{A}_i\left(\frac{\partial \mathbf{F}_j}{\partial x_j} + \frac{\partial \mathbf{G}_j}{\partial x_j} + \mathbf{Q}\right)\right] \tag{D.3c}$$

where $\mathbf{A}_i \equiv \partial \mathbf{F}_i / \partial \mathbf{\Phi}$.

If $\mathbf{Q} = \mathbf{Q}(\mathbf{\Phi}, x)$ and $\partial \mathbf{Q}/\partial \mathbf{\Phi} = \mathbf{S}$, then

$$\frac{\partial \mathbf{Q}}{\partial t} = \frac{\partial \mathbf{Q}}{\partial \mathbf{\Phi}}\frac{\partial \mathbf{\Phi}}{\partial t} = -\mathbf{S}\left(\frac{\partial \mathbf{F}_i}{\partial x_i} + \frac{\partial \mathbf{G}_i}{\partial x_i} + \mathbf{Q}\right) \tag{D.3d}$$

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and we can therefore approximate Eq. (D.2) as

$$\begin{aligned}\Delta\boldsymbol{\Phi}^n &\equiv \boldsymbol{\Phi}^{n+1}-\boldsymbol{\Phi}^n\\ &=-\Delta t\left[\frac{\partial \mathbf{F}_i}{\partial x_i}+\frac{\partial \mathbf{G}_i}{\partial x_i}+\mathbf{Q}\right]_n+\frac{\Delta t^2}{2}\left\{\frac{\partial}{\partial x_i}\left[\mathbf{A}_i\left(\frac{\partial \mathbf{F}_j}{\partial x_j}+\frac{\partial \mathbf{G}_j}{\partial x_j}+\mathbf{Q}\right)\right]\right.\\ &\quad\left.+\frac{\partial}{\partial t}\frac{\partial \mathbf{G}_i}{\partial x_i}+\mathbf{S}\left(\frac{\partial \mathbf{F}_j}{\partial x_j}+\frac{\partial \mathbf{G}_j}{\partial x_j}+\mathbf{Q}\right)\right\}_{n+\theta}\end{aligned}\tag{D.4}$$

Omitting the second derivatives of $\mathbf{G}_i$ and interpolating the $n+\theta$ between n and $n+1$ values and applying $n+\theta$ to $\mathbf{G}_i$ term we have

$$\begin{aligned}\Delta\boldsymbol{\Phi} &\equiv \boldsymbol{\Phi}^{n+1}-\boldsymbol{\Phi}^n\\ &=-\Delta t\left[\frac{\partial \mathbf{F}_i}{\partial x_i}+\mathbf{Q}\right]_n-\Delta t\left(\left[\frac{\partial \mathbf{G}_i}{\partial x_i}\right]_{n+1}\theta+\left[\frac{\partial \mathbf{G}_i}{\partial x_i}\right]_n(1-\theta)\right)\\ &\quad+\frac{\Delta t^2}{2}\left[\frac{\partial}{\partial x_i}\left\{\mathbf{A}_i\left(\frac{\partial \mathbf{F}_j}{\partial x_j}+\mathbf{Q}\right)\right\}+\mathbf{S}\left(\frac{\partial \mathbf{F}_j}{\partial x_j}+\mathbf{Q}\right)\right]_{n+1}\theta\\ &\quad+\frac{\Delta t^2}{2}\left[\frac{\partial}{\partial x_i}\left\{\mathbf{A}_i\left(\frac{\partial \mathbf{F}_j}{\partial x_j}+\mathbf{Q}\right)\right\}+\mathbf{S}\left(\frac{\partial \mathbf{F}_j}{\partial x_j}+\mathbf{Q}\right)\right]_n(1-\theta)\end{aligned}\tag{D.5}$$

At this stage a standard Galerkin approximation is applied which will result in a discrete, time-stepping scheme. As the explicit form is of particular interest we shall only give the details of the discretization process for $\theta=0$. Writing as usual

$$\boldsymbol{\Phi}\approx\mathbf{N}\tilde{\boldsymbol{\Phi}}$$

we have

$$\begin{aligned}\left(\int_\Omega \mathbf{N}^{\mathrm{T}}\mathbf{N}\mathrm{d}\Omega\right)\Delta\tilde{\boldsymbol{\Phi}} &=-\Delta t\left[\int_\Omega \mathbf{N}^{\mathrm{T}}\left(\frac{\partial \mathbf{F}_i}{\partial x_i}+\frac{\partial \mathbf{G}_i}{\partial x_i}+\mathbf{Q}\right)\mathrm{d}\Omega\right.\\ &\quad-\frac{\Delta t}{2}\int_\Omega \mathbf{N}^{\mathrm{T}}\frac{\partial}{\partial x_i}\left\{\mathbf{A}_i\left(\frac{\partial \mathbf{F}_j}{\partial x_j}+\frac{\partial \mathbf{G}_j}{\partial x_j}+\mathbf{Q}\right)\right\}\mathrm{d}\Omega\\ &\quad\left.-\frac{\Delta t}{2}\int_\Omega \mathbf{N}^{\mathrm{T}}\mathbf{S}\left(\frac{\partial \mathbf{F}_j}{\partial x_j}+\frac{\partial \mathbf{G}_j}{\partial x_j}+\mathbf{Q}\right)\mathrm{d}\Omega\right]_n\end{aligned}\tag{D.6}$$

This can be written in a compact matrix form similar to Eq. (2.107) as

$$\mathbf{M}\Delta\tilde{\boldsymbol{\Phi}}=-\Delta t[(\mathbf{C}+\mathbf{K}_u+\mathbf{K})\tilde{\boldsymbol{\Phi}}+\mathbf{f}]^n\tag{D.7a}$$

in which, with

$$\mathbf{G}_i=-k_{ij}\frac{\partial\boldsymbol{\Phi}}{\partial x_j}$$

we have (on omitting the third derivative terms and the effect of **S**) matrices of the form of Eq. (2.108), i.e.,

$$\begin{aligned}
\mathbf{C} &= \int_\Omega \mathbf{N}^{\mathrm{T}} \mathbf{A}_i \frac{\partial \mathbf{N}}{\partial x_i} \mathrm{d}\Omega \\
\mathbf{K}_u &= \int_\Omega \frac{\partial \mathbf{N}^{\mathrm{T}}}{\partial x_i} \left(\mathbf{A}_i \mathbf{A}_j \frac{\Delta t}{2} \right) \frac{\partial \mathbf{N}}{\partial x_j} \mathrm{d}\Omega \\
\mathbf{K} &= \int_\Omega \frac{\partial \mathbf{N}^{\mathrm{T}}}{\partial x_i} k_{ij} \frac{\partial \mathbf{N}}{\partial x_j} \mathrm{d}\Omega \\
\mathbf{f} &= \int_\Omega \left(\mathbf{N}^{\mathrm{T}} + \frac{\Delta t}{2} \mathbf{A}_i \frac{\partial \mathbf{N}^{\mathrm{T}}}{\partial x_i} \right) \mathbf{Q} \mathrm{d}\Omega + \text{boundary terms} \\
\mathbf{M} &= \int_\Omega \mathbf{N}^{\mathrm{T}} \mathbf{N} \mathrm{d}\Omega
\end{aligned} \tag{D.7b}$$

With $\theta = 1/3$ it can be shown that the order of approximation increases and for this scheme a simple iterative solution is possible [3]. We note that with the consistent mass matrix **M** the stability limit for $\theta = 1/3$ is increased to $C = 1$.

Use of $\theta = 1/3$ apparently requires an implicit solution. However, similar iteration to that used in Eq. (2.118) is rapidly convergent and the scheme can be used quite economically.

D.2 Two-step predictor-corrector methods: Two-step Taylor-Galerkin operation

There are of course various alternative procedures for improving the temporal approximation other than the Taylor expansion used in the previous section. Such procedures will be particularly useful if the evaluation of the derivative matrix $\mathbf{A}_i$ can be avoided. In this section we shall consider two predictor-corrector schemes (of the Runge-Kutta type) that avoid the evaluation of this matrix and are explicit.

The first starts with a standard Galerkin space approximation being applied to the basic Eq. (D.1). This results in the form

$$\mathbf{M} \frac{\mathrm{d}\tilde{\mathbf{\Phi}}}{\mathrm{d}t} \equiv \mathbf{M}\, \dot{\tilde{\mathbf{\Phi}}} = \mathbf{P}_C + \mathbf{P}_D + \mathbf{f} = \mathbf{\Psi} \tag{D.8}$$

where again **M** is the standard mass matrix, **f** the prescribed "forces," and

$$\mathbf{P}_C(\mathbf{\Phi}) = \int_\Omega \mathbf{N}^{\mathrm{T}} \frac{\partial \mathbf{F}_i}{\partial x_i} \mathrm{d}\Omega \tag{D.9a}$$

represents the convective "forces," while

$$\mathbf{P}_D(\mathbf{\Phi}) = \int_\Omega \mathbf{N}^{\mathrm{T}} \frac{\partial \mathbf{G}_i}{\partial x_i} \mathrm{d}\Omega \tag{D.9b}$$

are the diffusive ones.

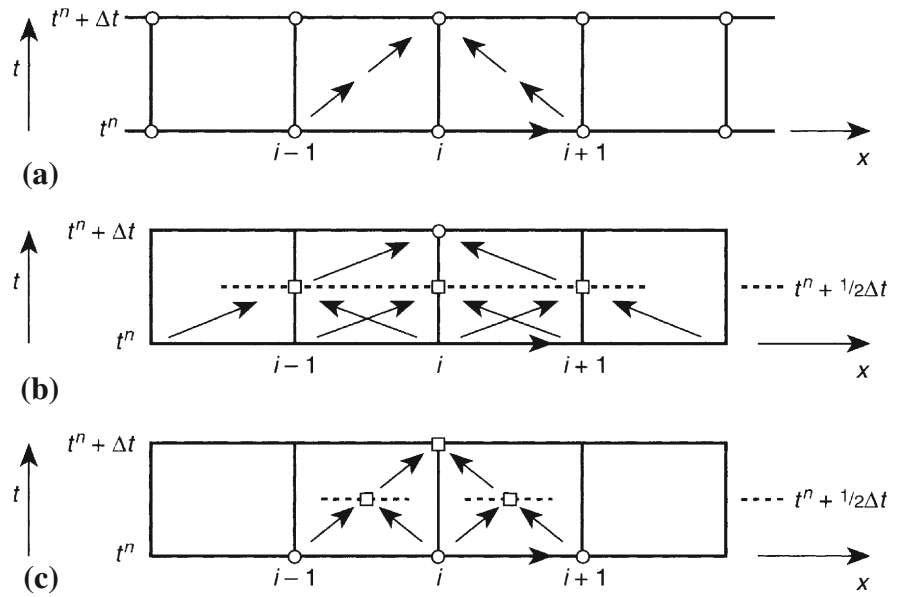

FIGURE D.1

Progression of information in explicit one- and two-step schemes: (a) single-step explicit; (b) standard predictor-corrector; (c) local predictor-corrector (two-step Taylor-Galerkin).

If an explicit time integration scheme is used, i.e.,

$$\mathbf{M}\Delta\boldsymbol{\Phi} \equiv \mathbf{M}(\tilde{\boldsymbol{\Phi}}^{n+1} - \tilde{\boldsymbol{\Phi}}^{n}) = \Delta t\,\boldsymbol{\Psi}^{n} \tag{D.10}$$

the evaluation of the right-hand side does not require the matrix product representation and $\mathbf{A}_i$ does not have to be computed.

Of course the scheme presented is not accurate for the various reasons previously discussed, and indeed becomes *unconditionally unstable* in the absence of diffusion and external force vectors.

The reader can easily verify that in the case of the linear one-dimensional problem the right-hand side is equivalent to a central difference scheme with $\tilde{\boldsymbol{\Phi}}^{n}_{i-1}$ and $\tilde{\boldsymbol{\Phi}}^{n}_{i+1}$ only being used to find the value of $\boldsymbol{\Phi}^{n+1}_{i}$, as shown in Fig. D.1a.

The scheme can, however, be recast as a two-step, predictor-corrector operation and conditional stability is regained. Now we proceed as follows:

Step 1. Compute $\tilde{\boldsymbol{\Phi}}^{n+1/2}$ using an explicit approximation of Eq. (D.10), i.e.,

$$\tilde{\boldsymbol{\Phi}}^{n+1/2} = \tilde{\boldsymbol{\Phi}}^{n} + \frac{\Delta t}{2}\mathbf{M}^{-1}\boldsymbol{\Psi}^{n} \tag{D.11}$$

and

Step 2. Compute $\tilde{\boldsymbol{\Phi}}^{n+1}$ inserting the improved value of $\tilde{\boldsymbol{\Phi}}^{n+1/2}$ in the right-hand side of Eq. (D.10), giving

$$\tilde{\boldsymbol{\Phi}}^{n+1} = \tilde{\boldsymbol{\Phi}}^{n} + \Delta t \mathbf{M}^{-1} \boldsymbol{\Psi}^{n+1/2} \tag{D.12}$$

This is precisely equivalent to the second-order Runge-Kutta scheme being applied to the ordinary system of differential equations (D.8). Figure D.1b shows in the one-dimensional example how the information "spreads," i.e., that now $\tilde{\boldsymbol{\Phi}}_i^{n+1}$ will be dependent on values at nodes $i-2, \ldots, i+2$.

It is found that the scheme, though stable, is overdiffusive and numerical results are poor.

An alternative is possible, however, using a two-step Taylor-Galerkin operation. Here we return to Eq. (D.1) and proceed as follows in semi-discrete form

Step 1. Find an improved value of $\boldsymbol{\Phi}^{n+1/2}$ *using only the convective and source parts*. Thus

$$\boldsymbol{\Phi}^{n+1/2} = \boldsymbol{\Phi}^{n} - \frac{\Delta t}{2}\left(\frac{\partial \mathbf{F}_i^n}{\partial x_i} + \mathbf{Q}^n\right) \tag{D.13a}$$

which of course allows the evaluation of $\mathbf{F}_i^{n+1/2}$.

We note, however, that we can also write an approximate expansion as

$$\begin{aligned}\mathbf{F}_i^{n+1/2} &= \mathbf{F}_i^n + \frac{\Delta t}{2}\frac{\partial \mathbf{F}_i^n}{\partial t} = \mathbf{F}_i^n - \frac{\Delta t}{2}\mathbf{A}_i^n \frac{\partial \boldsymbol{\Phi}^n}{\partial t} \\ &= \mathbf{F}_i^n - \frac{\Delta t}{2}\mathbf{A}_i^n \left(\frac{\partial \mathbf{F}_j}{\partial x_j} + \frac{\partial \mathbf{G}_j}{\partial x_j} + \mathbf{Q}\right)^n\end{aligned} \tag{D.13b}$$

This gives

$$\mathbf{A}_i^n \left(\frac{\partial \mathbf{F}_j}{\partial x_j} + \frac{\partial \mathbf{G}_j}{\partial x_j} + \mathbf{Q}\right)^n = -\frac{2}{\Delta t}(\mathbf{F}_i^{n+1/2} - \mathbf{F}_i^n) \tag{D.13c}$$

Step 2. Substituting the above into the Taylor-Galerkin approximation of Eq. (D.6) we have

$$\begin{aligned}\mathbf{M}\Delta\tilde{\boldsymbol{\Phi}} = -\Delta t \Bigg[&\int_\Omega \mathbf{N}^{\mathrm{T}} \left(\frac{\partial \mathbf{F}_i}{\partial x_i} + \frac{\partial \mathbf{G}_i}{\partial x_i} + \mathbf{Q}\right)^n \mathrm{d}\Omega \\ &+ \int_\Omega \mathbf{N}^{\mathrm{T}} \frac{\partial}{\partial x_i}(\mathbf{F}_i^{n+1/2} - \mathbf{F}_i^n)\mathrm{d}\Omega + \int_\Omega \mathbf{N}^{\mathrm{T}} \mathbf{S}(\mathbf{F}_i^{n+1/2} - \mathbf{F}_i^n)\mathrm{d}\Omega \Bigg]\end{aligned} \tag{D.13d}$$

and after integration by parts of the terms with respect to the x_i derivatives we obtain simply

$$\mathbf{M}\Delta\tilde{\mathbf{\Phi}} = -\Delta t\left\{ -\int_\Omega \frac{\partial \mathbf{N}^{\mathrm{T}}}{\partial x_i}(\mathbf{F}_i^{n+1/2} + \mathbf{G}_i^n)\mathrm{d}\Omega + \int_\Omega \mathbf{N}^{\mathrm{T}}[\mathbf{Q} + \mathbf{S}(\mathbf{F}^{n+1/2} - \mathbf{F}^n)]\mathrm{d}\Omega + \int_\Gamma \mathbf{N}^{\mathrm{T}}(\mathbf{F}_i^{n+1/2} + \mathbf{G}_i^n)\mathbf{n}_i\mathrm{d}\Gamma \right\} \tag{D.14}$$

We note immediately that:

1. The above expression is identical to *using a standard Galerkin approximation on* Eq. (D.1) and an explicit step with $\mathbf{F}_i$ values updated by the simple Eq. (D.13a).
2. The final form of Eq. (D.14) does not require the evaluation of the matrices $\mathbf{A}_i$ resulting in substantial computation savings as well as yielding essentially the same results. Indeed, some omissions made in deriving Eq. (D.7a) did not occur now and presumably the accuracy is improved.
   A further practical point must be noted:
3. In nonlinear problems it is convenient to interpolate $\mathbf{F}_i$ directly in the finite element manner as
$$\mathbf{F}_i = \mathbf{N}\tilde{\tilde{\mathbf{F}}}_i$$
rather than to compute it as $\mathbf{F}_i(\tilde{\tilde{\mathbf{\Phi}}})$.

Thus the evaluation of $\mathbf{F}_i^{n+1/2}$ need only be made at the quadrature (integration) points within the element, and the evaluation of $\tilde{\tilde{\mathbf{\Phi}}}^{n+1/2}$ by Eq. (D.13a) is only done on such points. For a linear triangle element this reduces to a single evaluation of $\tilde{\mathbf{\Phi}}^{n+1/2}$ and $\mathbf{F}^{n+1/2}$ for each element at its barycenter, taking of course $\tilde{\mathbf{\Phi}}^{n+1/2}$ and $\mathbf{F}^{n+1/2}$ as the appropriate interpolation average there.

In the simple one-dimensional linear example the information progresses in the manner shown in Fig. D.1c. The scheme, which originated at Swansea, can be appropriately called the *Swansea two step* [4–14], and has found much use in the direct solution of compressible high-speed gas flow equations. We presented some of the results obtained by this procedure in Chapter 7. In Chapter 3 we discussed an alternative which is more general and has better performance. It is of interest to remark that the Taylor-Galerkin procedure can be used in contexts other than direct fluid mechanics. The procedure has been used efficiently by Morgan et al. [15] in solving electromagnetic wave problems.

D.2.1 Multiple wave speeds

When ϕ is a scalar variable, a single wave speed will arise in the manner in which we have already shown at the beginning of Part II of Chapter 2. When a vector variable is considered, the situation is very different and in general the number of wave speeds

will correspond to the number of variables. If we return to the general equation (D.1), we can write this in the form

$$\frac{\partial \mathbf{\Phi}}{\partial t} + \mathbf{A}_i \frac{\partial \mathbf{\Phi}}{\partial x_i} + \frac{\partial \mathbf{G}_i}{\partial x_i} + \mathbf{Q} = \mathbf{0} \tag{D.15}$$

where $\mathbf{A}_i$ is a matrix of the size corresponding to the variables in the vector $\tilde{\mathbf{\Phi}}$. This is equivalent to the single convective velocity component $A = U$ in a scalar problem and is given as

$$\mathbf{A}_i \equiv \frac{\partial \mathbf{F}_i}{\partial \mathbf{\Phi}} \tag{D.16}$$

This in general may still be a function of $\mathbf{\Phi}$, thus destroying the linearity of the problem.

Before proceeding further, it is of interest to discuss the general behavior of Eq. (D.1) in the absence of source and diffusion terms. We note that the matrices $\mathbf{A}_i$ can be represented as

$$\mathbf{A}_i = \mathbf{X}_i \mathbf{\Lambda}_i \mathbf{X}_i^{-1} \tag{D.17}$$

by a standard eigenvalue analysis in which $\mathbf{\Lambda}_i$ is a diagonal matrix.

If the eigenvector matrices $\mathbf{X}_i$ are such that

$$\mathbf{X}_i = \mathbf{X} \tag{D.18}$$

which is always the case in a single dimension, then Eq. (D.15) can be written (in the absence of diffusion or source terms) as

$$\frac{\partial \mathbf{\Phi}}{\partial t} + \mathbf{X} \mathbf{\Lambda}_i \mathbf{X}^{-1} \frac{\partial \mathbf{\Phi}}{\partial x_i} = \mathbf{0} \tag{D.19}$$

Premultiplying by $\mathbf{X}^{-1}$ and introducing new variables (called Riemann invariants) such that

$$\boldsymbol{\phi} = \mathbf{X}^{-1} \mathbf{\Phi} \tag{D.20}$$

we can write the above as a set of decoupled equations in components ϕ of $\mathbf{\Phi}$ and corresponding Λ of $\mathbf{\Lambda}$:

$$\frac{\partial \phi}{\partial t} + \Lambda_i \frac{\partial \phi}{\partial x_i} = 0 \tag{D.21}$$

each of which represents a wave-type equation of the form that we have previously discussed. A typical example of the above results from a one-dimensional elastic dynamics problem describing stress waves in a bar in terms of stresses (σ) and velocities (v) as

$$\frac{\partial \sigma}{\partial t} - E \frac{\partial v}{\partial x} = 0$$
$$\frac{\partial v}{\partial t} - \frac{1}{\rho} \frac{\partial \sigma}{\partial x} = 0$$

This can be written in the standard form of Eq. (D.1) with

$$\mathbf{\Phi} = \begin{Bmatrix} \sigma \\ v \end{Bmatrix} \qquad \mathbf{F} = \begin{Bmatrix} E v \\ \sigma/\rho \end{Bmatrix}$$

The two variables of Eq. (D.20) become

$$\phi_1 = \sigma - c\, v \qquad \text{and} \qquad \phi_2 = \sigma + c\, v$$

where $c = \sqrt{E/\rho}$ and the equations corresponding to (D.21) are

$$\frac{\partial \phi_1}{\partial t} + c\,\frac{\partial \phi_1}{\partial x} = 0$$
$$\frac{\partial \phi_2}{\partial t} - c\,\frac{\partial \phi_2}{\partial x} = 0$$

representing respectively two waves moving with velocities $\pm c$.

Unfortunately the condition of Eq. (D.18) seldom pertains and hence the determination of general characteristics and therefore decoupling is not usually possible for more than one space dimension. This is the main reason why the extension of the simple, direct procedures is not generally possible for vector variables. Because of this in Chapter 3 we only used the upwinding characteristic-based procedures on scalar systems for which a single wave speed exists and this retains justification of any method proposed.

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