Appendix A

Introduction to the Finite Volume Code

The aim of this appendix is to introduce the underlying ideas that form the basis of the hydrodynamic model used in Chapter 3. The intent is not to provide an extensive discussion, but merely to sketch the basic outlines of the principles involved. The introduction presented in this appendix largely follows the presentation of LeVeque (2002), where a more thorough treatment of this subject can be found. Although not as extensive as LeVeque (2002), the textbooks of, e.g., Lomax et al. (2001) and Chattot (2002) provide an equally good overview of this topic. As part of this introduction to the model, its history is also reviewed.

For the sake of simplicity, the introduction presented in this section focuses on a one-dimensional scenario. However, the ideas presented here can easily be extended to additional dimensions. Furthermore, the discussion is presented for a general system of hyperbolic equations, of which the Euler equations (3.1) are but a single example. For a discussion on how the present formulation specifically relates to the Euler equations, Snyman (2007) can be consulted.

The Euler equations (3.1) are an example of a non-linear system of equations

\[ q_t(x,t) + f(q(x,t))_x = 0 \]  
(A.1)

that can alternatively be rewritten in the quasi-linear form

\[ q_t + f'(q)q_x = 0, \]  
(A.2)

where \( q : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}^m \) is a vector with \( m \) components containing the unknown scalar quantities, and \( f'(q) = \partial f/\partial q \) is defined as a constant \( m \times m \) real matrix. For the Euler equations, a comparison with (3.1) shows that

\[
q = \begin{bmatrix}
\rho \\
\rho V \\
E
\end{bmatrix} 
\]  
(A.3a)

and

\[
f'(q) = \begin{bmatrix}
0 & 1 & 0 \\
\frac{1}{2} (\gamma - 3) V^2 & (3 - \gamma) V & \gamma - 1 \\
\frac{1}{2} (\gamma - 1) V^3 - VH & H - (\gamma - 1) V^2 & \gamma V
\end{bmatrix}, 
\]  
(A.3b)
where
\[ E = \frac{P}{\gamma - 1} + \frac{1}{2} \rho V^2 \] \hspace{1cm} (A.4a)
represents the total energy density of the fluid, and
\[ H = \frac{E + P}{\rho} \] \hspace{1cm} (A.4b)
the total specific enthalpy.

For a hyperbolic system of equations such as (A.2), finite volume methods are often the preferred numerical solution technique. Before briefly discussing these numerical methods, it is necessary to first introduce a few concepts.

A.1 The advection equation

For the case \( m = 1 \), the matrix \( f'(q) \) reduces to a single scalar value. As it is assumed that this scalar quantity is a constant, the system of equations (A.2) is simplified to the single linear advection (convection) equation
\[ q_t(x, t) + \bar{u} q_x(x, t) = 0. \] \hspace{1cm} (A.5)
The general solution to (A.5) can easily be calculated, and is found to be of the form
\[ q(x, t) = \tilde{q}(x - \bar{u} t) \] \hspace{1cm} (A.6)
for any function \( \tilde{q}(x, t) \). The initial concentration (or waveform) specified by \( \tilde{q} \) propagates with unaltered shape and constant speed \( |\bar{u}| \). The wave propagates towards the right if \( \bar{u} \) is positive, and towards the left if \( \bar{u} \) is negative. It may alternatively be stated that \( q \) is constant along the characteristic curves \( x - \bar{u} t \) in the \((x, t)\)-plane (cf. Section 5.2.3).

A.2 The wave propagation approach

The numerical technique used for the simulations in Chapter 3 is based on a wave propagation approach, and follows from the hyperbolic nature of the Euler equations (3.1). To illustrate the basic idea, consider the system of linear equations (A.2). The system is said to be hyperbolic if the \( m \times m \) matrix \( f'(q) \) can be diagonalised with real eigenvalues, denoted by
\[ \lambda^1 \leq \lambda^2 \leq \ldots \lambda^m. \]
The \( m \times m \) matrix \( f'(q) \) can be diagonalised if and only if it possesses a set of \( m \) linearly independent eigenvectors \( r^1, r^2, \ldots, r^2 \in \mathbb{R}^2 \) such that (see, e.g., Johnson et al., 2002)
\[ f'(q)r^p = \lambda^p r^p \quad \text{for} \quad p = 1, 2, \ldots, m. \] \hspace{1cm} (A.7)
To prove that $f'(q)$ is diagonalisable, form the matrix $R$ by collecting the eigenvectors into a single matrix, i.e.

$$R = \begin{bmatrix} r^1 & r^2 & \ldots & r^m \end{bmatrix}.$$  \hfill (A.8)

Because the matrix $R$ is nonsingular, the inverse matrix $R^{-1}$ exists, thereby allowing one to write (see, e.g., Johnson et al., 2002)

$$R^{-1} f'(q) R = \Lambda \quad \text{and} \quad f'(q) = R \Lambda R^{-1},$$  \hfill (A.9)

where

$$\Lambda = \begin{bmatrix} \lambda^1 & & & \\ & \lambda^2 & & \\ & & \ddots & \\ & & & \lambda^m \end{bmatrix} \equiv \text{diag} (\lambda^1, \lambda^2, \ldots, \lambda^m).$$  \hfill (A.10)

It thus follows that the matrix $f'(q)$ is similar to the diagonal matrix $\Lambda$, i.e. they have the same eigenvalues (see, e.g., Johnson et al., 2002).

The importance of the last statement can be understood by rewriting (A.2) as

$$R^{-1} q_t + R^{-1} f'(q) R R^{-1} q_x = 0.$$  \hfill (A.11)

Defining $w(x,t) \equiv R^{-1} q(x,t)$, the above equation can be written as

$$w_t + \Lambda w_x = 0.$$  \hfill (A.12)

Because $\Lambda$ is diagonal, the initial system of linear differential equations (A.2) has decoupled into $m$ independent advection equations for the components $w^p$ of $w$:

$$w^p_t + \lambda^p w^p_x = 0 \quad \text{for} \quad p = 1, 2, \ldots, m.$$  \hfill (A.13)

Similar to the advection equation (A.5), information in this decoupled set of advection equations (A.13) will propagate along the characteristic curves $x(t) = x_0 + \lambda^p t$. Once the components $w^p$ are known, they can be collected in the vector $w(x,t)$, with the solution to the original problem then given by

$$q(x,t) = R w(x,t) = \begin{bmatrix} r^1 & r^2 & \ldots & r^m \end{bmatrix} \begin{bmatrix} w^1 \\ w^2 \\ \vdots \\ w^m \end{bmatrix}.$$  \hfill (A.14)

The solution

$$q(x,t) = \sum_{p=1}^{m} w^p(x,t) r^p$$  \hfill (A.15)

will therefore consist of a superposition of $m$ independent waves travelling at the characteristic speeds $\lambda^1 \leq \lambda^2 \leq \ldots \lambda^m$. 

The definition of a hyperbolic system can easily be extended to systems with variable coefficients

\[ q_t + f'(q)q_x = 0. \]  \hspace{1cm} (A.16)

In this case the system is hyperbolic at any point \( x \) where \( f'(q) \) can be diagonalised with real eigenvalues.

### A.3 The Riemann problem

The Riemann problem is defined as a hyperbolic system of equations, such as (A.2), with initial data that are piecewise constant, i.e. separated by a jump discontinuity

\[ \tilde{q}(x) = \begin{cases} q_l, & \text{if } x \leq 0 \\ q_r, & \text{if } x > 0 \end{cases}. \]  \hspace{1cm} (A.17)

Invoking (A.15), the data at \( x \leq 0 \) and \( x > 0 \) can be decoupled as

\[ q_l = \sum_{p=1}^{m} w^p_l r^p \text{ and } q_r = \sum_{p=1}^{m} w^p_r r^p. \]  \hspace{1cm} (A.18)

Note that the difference in \( \tilde{q}(x) \) on the opposite sides of \( x = 0 \) is contained in the values of the \( w^p_l \) and \( w^p_r \) as it is assumed that the eigenvectors \( r^p \) are spatially independent. Comparison of (A.17) with (A.18) shows that one may write the initial conditions of the components \( w^p \) as

\[ \tilde{w}^p(x) = \begin{cases} w^p_l, & \text{if } x \leq 0 \\ w^p_r, & \text{if } x > 0 \end{cases}. \]  \hspace{1cm} (A.19)

Now, for an advection equation of the form

\[ w_t + \lambda w_x = 0, \]  \hspace{1cm} (A.20)

with the initial condition \( w(x,0) = \tilde{w}(x) \), it was stated in Section A.1 that the quantity \( \tilde{w}(x) \) simply advects along \( x \) with a velocity \( \lambda \). In the context of the Riemann problem this implies that the \( p \)th discontinuity in (A.19) advects along \( x \) with a velocity given by the \( p \)th eigenvalue \( \lambda^p \) of \( f'(q) \). Therefore, the solution to (A.20) is given by

\[ w^p(x,t) = \begin{cases} w^p_l, & \text{if } x - \lambda^p t \leq 0 \\ w^p_r, & \text{if } x - \lambda^p t > 0 \end{cases}, \]  \hspace{1cm} (A.21)

and subsequently it follows from (A.15) that the solution of the system is given by

\[ q(x,t) = \sum_{p: \lambda^p < x/t} w^p_l r^p + \sum_{p: \lambda^p \geq x/t} w^p_r r^p. \]  \hspace{1cm} (A.22)
A.4 Finite volume methods

As discussed in, e.g., Lomax et al. (2001) and LeVeque (2002), the starting point of all finite volume methods is the integral form

$$\frac{d}{dt} \int_{x_1}^{x_2} q(x,t) dx = f(q(x,t)) \bigg|_{x_1}^{x_2}$$  \hspace{1cm} (A.23)

of the conservation equation (A.1). In the derivation of (A.1) it is assumed that \( q(x,t) \) is continuous for all values of \( x \) and \( t \), whereas the integral formulation (A.23) makes no such assumption. Finite volume methods are thus ideal for simulating systems with discontinuities, most notably systems where shocks are expected to form.

To construct the numerical scheme, the computational domain is first divided into a number of cells, or volume elements, with a cell occupying the part of the domain that extends between \( x_i \) and \( x_{i+1} \), for \( i = 0, 1, \ldots, n \). Next, the average value of \( q(x,t) \) in the \( i \)th cell at a time \( t_n \) is calculated using

$$Q_{i+1/2} \approx \frac{1}{\Delta x} \int_{x_i}^{x_{i+1}} q(x, t_n) dx.$$  \hspace{1cm} (A.24)

For data that is initially smooth, the averaging procedure will lead to data that is piecewise constant between neighbouring cells. In essence, the problem has therefore been reduced to solving the Riemann problem at every cell interface. Using (A.15), the difference between the various cells can be written as

$$Q_{i+1/2}^n - Q_{i-1/2}^n = \sum_{p=1}^{m} \left( w_{i+1/2}^p - w_{i-1/2}^p \right) r^p.$$  \hspace{1cm} (A.25)

Integrating (A.23) over time, and dividing the result by the cell width \( \Delta x \), leads to

$$Q_{i+1/2}^{n+1} = Q_{i+1/2}^n - \frac{\Delta t}{\Delta x} \left( F_{i+1}^n - F_i^n \right),$$  \hspace{1cm} (A.26)

where

$$F_i^n \approx \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} f(q(x,t)) \, dt$$  \hspace{1cm} (A.27)

is an approximation of the average flux through the cell interface at \( x = x_i \). If the average flux can be based on the values of \( Q^n \), then a fully discreet method can be obtained (see, e.g., LeVeque, 2002).

A.5 The development of the code

The numerical code was initially developed by Kausch (1998), and is based on a five-fluid, axisymmetric hydrodynamic model of the heliosphere. This development of the code formed the basis of the above-mentioned author’s doctoral research, and a detailed derivation of the numerical scheme, as well as a discussion of possible numerical intricacies, can be found in
Kausch (1998). This version of the code was also later used by Fahr et al. (2000) to model the interaction between the heliosphere and the interstellar medium.

In the initial iteration, the five-fluid model contained two non-thermal fluid components (galactic and anomalous cosmic rays) that were approximately treated as thermal components. In an extension of the model, Scherer and Ferreira (2005a) calculated the evolution of the non-thermal particle spectra using the Parker (1965) transport equation, thereby making it possible to correctly calculate the changes in fluid pressure as a result of these particles, with this component eventually constituting part of the total pressure. In this form, the model was used by Scherer and Ferreira (2005b) and Ferreira and Scherer (2006) to explain the observed cosmic ray intensities.

A simpler three-fluid version of the code was used by Snyman (2007) to study the effect of different parameters on the evolution of a dynamical heliosphere. This formed the topic of research for the author’s Masters dissertation, where a very decent introduction to the numerical scheme can be found. Not only is the appropriate finite volume method discussed in more detail than in this appendix, but it is also shown how the scheme is specifically derived for the Euler equations (3.1). A summary of the main results of Snyman (2007) can be found in Snyman et al. (2006).

Apart from modelling the heliosphere, the numerical model has also been applied to astrophysical systems. Simplifying the model so as to describe only a single fluid, Ferreira and de Jager (2008) included a kinematic treatment of the magnetic field, and used this modified version of the code to simulate the evolution of a supernova remnant in both a homogeneous and an inhomogeneous interstellar medium. This same model has also been used by Van den Heever (2011) to study the interaction between stellar winds and the interstellar medium, focusing on the effect that this interaction has on any subsequent supernova explosions.
Appendix B

The Transport Equation in Spherical Coordinates

In the first part of this appendix, the general transport equation is transformed into the spherical coordinates $r$, $\theta$, and $\phi$. Additionally, this transformation also shows the form of the momentum term in the transport equation when adiabatic cooling, synchrotron radiation/inverse Compton scattering, and momentum diffusion are taken into account. In the second part of this appendix, it is shown how the momentum term is modified when Klein-Nishina effects are taken into account.

B.1 Derivation of the transport equation

The general transport equation is given by

$$\frac{\partial f}{\partial t} + \nabla \cdot S - \frac{1}{p^2} \frac{\partial}{\partial p} \left( p^2 \left[ \langle \dot{p} \rangle f + D_p \frac{\partial f}{\partial p} \right] \right) = Q(r, p, t), \quad (B.1)$$

where

$$S = 4\pi p^2 (\mathbf{V} f - \mathbf{K} \cdot \nabla f). \quad (B.2)$$

The second term in (B.1), describing convection, can be expanded as

$$\nabla \cdot (\mathbf{V} f) = \mathbf{V} \cdot (\nabla f) + f (\nabla \cdot \mathbf{V})$$

$$= V_r \frac{\partial f}{\partial r} + \frac{V_\theta}{r} \frac{\partial f}{\partial \theta} + \frac{V_\phi}{r \sin \theta} \frac{\partial f}{\partial \phi} + (\nabla \cdot \mathbf{V}) f. \quad (B.3)$$

With the diffusion coefficient defined as

$$\mathbf{K} = \begin{bmatrix} \kappa_{rr} & \kappa_{r\theta} & \kappa_{r\phi} \\ \kappa_{\theta r} & \kappa_{\theta\theta} & \kappa_{\theta\phi} \\ \kappa_{\phi r} & \kappa_{\phi\theta} & \kappa_{\phi\phi} \end{bmatrix},$$
the diffusive term in (B.2) can be expanded as

$$
\nabla \cdot (K \cdot \nabla f) =
\begin{align*}
&\kappa_{rr} \frac{\partial^2 f}{\partial r^2} + \kappa_{\theta\theta} \frac{\partial^2 f}{\partial \theta^2} + \frac{\kappa_{\phi\phi}}{r^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2} \\
&+ \left( \frac{r \kappa_{rr} + \kappa_{\theta\theta}}{r} \right) \frac{\partial^2 f}{\partial r \partial \theta} + \left( \frac{r \kappa_{\theta\phi} + \kappa_{\phi\theta}}{r \sin \theta} \right) \frac{\partial^2 f}{\partial r \partial \phi} + \left( \frac{r \kappa_{\phi\phi} + \kappa_{\theta\theta}}{r^2 \sin \theta} \right) \frac{\partial^2 f}{\partial \theta \partial \phi} \\
&+ \left[ \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \kappa_{rr}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \kappa_{\theta\theta}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} (\kappa_{\phi\theta}) \right] \frac{\partial f}{\partial r} \\
&+ \left[ \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial r} (r \kappa_{r\phi}) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \kappa_{\theta\phi}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} (\kappa_{\phi\phi}) \right] \frac{\partial f}{\partial \theta} \\
&+ \left[ \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial r} (r \kappa_{\phi\phi}) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} (\kappa_{\phi\phi}) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial}{\partial \phi} (\kappa_{\phi\phi}) \right] \frac{\partial f}{\partial \phi}.
\end{align*}
$$

The adiabatic cooling (heating) rate is given by

$$
\langle \dot{p}_{ad} \rangle = \frac{1}{3} \nabla \cdot \mathbf{V},
$$

while the energy loss rate for the non-thermal processes of synchrotron radiation and inverse Compton scattering is given by (see, e.g., Longair, 2011)

$$
\langle \dot{E}_{n-t} \rangle = \frac{4}{3} \sigma T c \beta^2 \gamma^2 U_i,
$$

where \( \beta \) and \( \gamma \) are the usual relativistic factors. The variable \( U_i(r, t) \) represents the energy density of the target photon field \( U_{1C} \), or in the case of synchrotron radiation, the energy density of the magnetic field \( U_B \). The transformation of the energy loss rate into a momentum loss rate starts with the well-known energy equation for a relativistic particle

$$
E = \sqrt{(pc)^2 + E_0^2},
$$

from which it follows that

$$
\frac{dE}{dp} = \frac{pc^2}{\sqrt{(pc)^2 + E_0^2}}. \tag{B.7}
$$

The next step is to rewrite \( \beta^2 \gamma^2 \) in (B.6) as a function of \( p \). Taking the expression for relativistic momentum, dividing by the speed of light \( c \), and squaring the resulting expression, leads to

$$
p = \gamma m_0 v \Rightarrow \frac{p}{c} = \gamma m_0 v c = \gamma m_0 \beta \Rightarrow \frac{p^2}{m_0 c^2} = \gamma^2 \beta^2. \tag{B.8}
$$

The desired momentum loss rate can be obtained by inserting (B.7) and (B.8) into

$$
\langle \dot{E}_{n-t} \rangle = \frac{dE}{dp} \frac{dp}{dt},
$$
which, after some slight mathematical manipulation, leads to

\[
\langle \dot{p} \rangle_{n-t} = \frac{4}{3} \sigma_T \frac{c p}{E_0} \sqrt{(pc)^2 + E_0^2} \left( U_B + U_{1C} \right).
\]

For particles with \( E \gg E_0 \), the momentum loss rate simplifies to

\[
\langle \dot{p} \rangle_{n-t} = z_p p^2,
\]  

(B.9)

with

\[
z_p = \frac{4}{3} \sigma_T \frac{1}{(m_0 c)^2} U_B \left( 1 + \frac{U_{1C}}{U_B} \right).
\]

Inserting (B.5) and (B.9) into the transport equation (B.1), while defining the total momentum
loss rate as \( \langle \dot{p} \rangle_{tot} = \langle \dot{p} \rangle_{syn} + \langle \dot{p} \rangle_{adv} \), leads to

\[
\frac{1}{p^2} \frac{\partial}{\partial p} \left( \langle \dot{p} \rangle_{tot} p^2 f \right) = \frac{z_p p^4}{p^2} \frac{\partial f}{\partial p} + \frac{z_p f}{p^2} \frac{\partial}{\partial p} \left( p^4 \right) + \frac{(\nabla \cdot \mathbf{V})}{3} \frac{\partial f}{\partial p} + (\nabla \cdot \mathbf{V}) f,
\]  

(B.10)

where

\[
\frac{(\nabla \cdot \mathbf{V})}{3} \frac{\partial f}{\partial p} = \frac{1}{3} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 V_r \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta V_\theta \right) + \frac{1}{r \sin \theta} \frac{\partial V_\phi}{\partial \phi} \right] \frac{p^2}{\partial p}. \]

(B.11)

Note that the term \((\nabla \cdot \mathbf{V}) f\) in (B.10) cancels with the last term of (B.3).

Assuming that the spatial and momentum dependence of the momentum diffusion coefficient are separable so that \( D_p = \kappa_p (r, t, p) \) (see, e.g., Lerche and Schlickeiser, 1981), the momentum diffusion term in (B.1) can be written as

\[
\frac{1}{p^2} \frac{\partial}{\partial p} \left[ (\kappa_p p^4) \frac{\partial f}{\partial p} \right] = \frac{4 \kappa_p p^3}{p^2} \frac{\partial f}{\partial p} + \frac{\kappa_p p^4 \partial^2 f}{p^2} = 4 \kappa_p \frac{\partial f}{\partial \ln p} + \kappa_p \frac{\partial^2 f}{\partial \ln p^2} - \kappa_p \frac{\partial f}{\partial \ln p}.
\]  

(B.12)

Inserting (B.3), (B.4), (B.10), and (B.12) into (B.1), and grouping all the appropriate terms, leads to the transport equation

\[
\frac{\partial f}{\partial t} = \kappa_{rr} \frac{\partial^2 f}{\partial r^2} + \kappa_{r\theta} \frac{\partial^2 f}{\partial r \partial \theta} + \kappa_{\phi \theta} \frac{\partial^2 f}{\partial \theta^2} + \kappa_p \frac{\partial^2 f}{\partial \ln p^2} + \left( \frac{\kappa_{r\theta}}{r} \frac{\partial^2 f}{\partial r \partial \theta} + \left( \frac{\kappa_{r\phi}}{r^2 \sin \theta} \frac{\partial^2 f}{\partial \theta^2} + \kappa_p \frac{\partial^2 f}{\partial \ln p^2} + \left( \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \kappa_{rr} \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \kappa_{r\theta} \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \left( \kappa_{r\phi} \right) - V_r \frac{\partial f}{\partial r} \right)
+ \left( \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial r} \left( r \kappa_{r\theta} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \kappa_{\phi \theta} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \phi} \left( \kappa_{\phi \theta} \right) - V_\phi \frac{\partial f}{\partial \theta} \right)
+ \left( \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial r} \left( r \kappa_{r\phi} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \kappa_{\phi \theta} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \phi} \left( \kappa_{\phi \phi} \right) - V_\phi \frac{\partial f}{\partial \phi} \right)
+ \frac{1}{3} \left( \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 V_r \right) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta V_\theta \right) + \frac{1}{r \sin \theta} \frac{\partial V_\phi}{\partial \phi} + 3 z_p p + 9 \kappa_p \right) \frac{\partial f}{\partial \ln p} \right)
+ 4 z_p p f
+ Q \left( r, \theta, \phi, p, t \right).
\]  

(B.13)
Imposing an azimuthal symmetry on the system \((\partial/\partial \phi = 0)\) reduces (B.13) to

$$\frac{\partial f}{\partial t} = \kappa_r \frac{\partial^2 f}{\partial r^2} + \kappa_{\theta \theta} \frac{\partial^2 f}{\partial \theta^2} + \kappa_p \frac{\partial^2 f}{\partial \ln p^2} + \left( \frac{\kappa_{\theta \theta}}{r} \right) \frac{\partial^2 f}{\partial r \partial \theta} + \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \kappa_r \right) - V_r \right] \frac{\partial f}{\partial r} + \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r \kappa_{\theta \theta} \right) - V_{\theta \theta} \right] \frac{\partial f}{\partial \theta} + \left[ \frac{1}{3} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 V_r \right) - \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \kappa_{\theta \theta} \right) - 3z_p p + 9 \kappa_p \right] \frac{\partial f}{\partial \ln p} + 4z_p p f + Q \left( r, \theta, p, t \right).$$

(B.14)

If the problem is spherically symmetric \((\partial/\partial \phi, \partial/\partial \theta = 0)\), (B.13) can be further reduced to

$$\frac{\partial f}{\partial t} = \kappa_r \frac{\partial^2 f}{\partial r^2} + \kappa_p \frac{\partial^2 f}{\partial \ln p^2} + \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \kappa_r \right) - V_r \right] \frac{\partial f}{\partial r} + \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \kappa_{\theta \theta} \right) + 3z_p p + 9 \kappa_p \right] \frac{\partial f}{\partial \ln p} + 4z_p p f + Q \left( r, p, t \right).$$

(B.15)

### B.2 The Klein-Nishina correction

The momentum loss rate as a result of inverse Compton scattering for an isotropic distribution of relativistic particles is given by

$$\langle \dot{p} \rangle_{IC} = \frac{4}{3} \sigma_T \frac{p^2}{(m_0 c)^2} U_{IC} F_{KN},$$

(B.16)

with the Klein-Nishina correction taken into account with the factor \(F_{KN}\). In the Thomson limit \(F_{KN} = 1\), while Moderski et al. (2005) have shown that this factor can be approximated as

$$F_{KN} \simeq \frac{1}{(1 + \Sigma)^{\alpha_{KN}}}$$

(B.17)

when the scattering occurs in the Klein-Nishina limit. The power-law index \(\alpha_{KN}\) appearing in this approximation is dependent on the energy spectrum of the target photons, while \(\Sigma = 4\gamma \epsilon\), with the energy of the target photons expressed in terms of the particle’s rest mass \(\epsilon = h\nu/m_0 c^2\).

Moderski et al. (2005) have shown that it is possible to find approximations to \(F_{KN}\) in the Klein-Nishina limit for the following energy distributions of the target photon field, \(u_\epsilon \propto \epsilon^{-\alpha_{KN}}\):
Mono-energetic spectrum: if \( E_e \lesssim 10^4 \), then the approximation

\[
F_{KN} \simeq \frac{1}{(1 + E_e)^{1.5}}
\]  
(B.18a)
can be used. It is possible to approximate a Planck-spectrum as a mono-energetic photon field by setting \( E_e = 4\gamma\epsilon_{\text{max}} \), where \( \epsilon_{\text{max}} = 2k_B T \), with \( k_B \) being Boltzmann’s constant and \( T \) the temperature;

- \( \alpha_{KN} > 1 \): inverse Compton losses are dominated by the scattering of low energy photons, and the approximation (B.18a) can gain be used, with the difference that \( E_e = 4\gamma\epsilon_{\text{min}} \). If \( 4\gamma_{\text{max}}\epsilon_{\text{min}} < 1 \), then all scattering is effectively in the Thomson regime;

- \( 0 < \alpha_{KN} < 1 \): inverse Compton losses are dominated by the scattering of high energy photons, and the approximation is given by

\[
F_{KN} \simeq \frac{1}{(1 + E_e)^{1-\alpha_{KN}}},
\]  
(B.18b)
with \( E_e = 4\gamma\epsilon_{\text{max}} \).

Replacing \( \gamma = p/m_0c \), and defining

\[
\tilde{\epsilon} = \frac{4h\nu}{m_0c^2} \frac{1}{m_0c}
\]  
(B.19)
so that \( \Sigma = \tilde{\epsilon}p \), the inverse Compton momentum loss term in the transport equation becomes

\[
\frac{1}{p^2} \frac{\partial}{\partial p} \left[ (\dot{p})_{ICp^2f} \right] = \frac{1}{p^2} \frac{\partial}{\partial p} \left[ z_{KN}p^2 \frac{2}{(1 + \tilde{\epsilon}p)^{\alpha_{KN}}} \right],
\]  
(B.20)
where

\[
z_{KN} = \frac{4}{3 (m_0c)^2} \sigma_T U_{IC}.
\]
Expanding (B.20) leads to

\[
\frac{1}{p^2} \frac{\partial}{\partial p} \left[ (\dot{p})_{ICp^2f} \right] = \frac{z_{KN}}{(1 + \tilde{\epsilon}p)^{\alpha_{KN}}} \frac{\partial f}{\partial \ln p} + z_{KN}f \left[ \frac{4(1 + \tilde{\epsilon}p)^{\alpha_{KN}} - \alpha_{KN}\tilde{\epsilon}p (1 + \tilde{\epsilon}p)^{\alpha_{KN}-1}}{(1 + \tilde{\epsilon}p)^{2\alpha_{KN}}} \right] \]  
(B.21)
From (B.17) it follows that the Thomson limit is obtained by setting \( \alpha_{KN} = 0 \), reducing (B.21) to a form that is identical to the first two terms on the right-hand side of (B.10).
Appendix C

Parabolic Finite-Difference Schemes

Partial differential equations can often only be solved by making use of numerical methods. This appendix introduces the finite-difference methods that are used to solve the one and two-dimensional transport equations (B.15) and (B.14) presented in the previous appendix. These methods are then used to derive the appropriate numerical schemes for the above-mentioned equations.

C.1 Classification of partial differential equations

Second-order linear partial differential equations can be expressed in the general form

$$\sum_{i,j} a_{ij}(x, u) u_{x,x} + \sum_{i} b_i(x, u) u_{x} + c(x, u) = 0.$$  (C.1)

Assuming that the coefficients $a_{ij}, b_i$ and $c$ are real, it is possible to divide the above equation into a number of subclasses using the eigenvalues of the coefficient matrix $A = [a_{ij}]$. If the condition $u_{x,x} = u_{x,x}$ holds, it follows that $A$ is an $n \times n$ symmetrical matrix with $n$ real eigenvalues. The partial differential equation is said to be

- **elliptic** if the eigenvalues are all positive or all negative;
- **parabolic** if the eigenvalues are all positive or all negative, with the exception of a single null eigenvalue;
- **hyperbolic** if the eigenvalues are all positive with the exception of a single negative eigenvalue, or vice versa;
- **ultra-hyperbolic** if there are multiple positive and negative eigenvalues without any null eigenvalues.

It is important to determine the character of the partial differential equation, as this will often dictate the choice of numerical technique employed in its solution. While the above classification holds for both constant and non-constant coefficients, it should be noted that the latter
can lead to a partial differential equation that has a different character at various locations in
the region under consideration.

The transport equation (B.14) presented in the previous appendix has the coefficient matrix

\[
A = \begin{bmatrix}
0 & 0 & 0 & 0 \\
0 & a_{rr} & 0 & 0 \\
0 & 0 & a_{\theta\theta} & 0 \\
0 & 0 & 0 & a_{pp}
\end{bmatrix}.
\]  

(C.2)

The determinant of the triangular eigenvalue matrix \( \det (A - \lambda I) \) is given by the product of the
diagonal entries, leading to the polynomial

\[(a_{rr} - \lambda)(a_{\theta\theta} - \lambda)(a_{pp} - \lambda) \lambda = 0 \]

and eigenvalues \( \lambda = a_{rr}, a_{\theta\theta}, a_{pp}, 0 \). As the coefficients \( a_{ii} \) are always positive, the transport
equation has a parabolic character.

C.2 Finite difference approximations

C.2.1 Numerical approximations

The basic derivation of a finite-difference scheme can be found in many textbooks dealing with
numerical methods, including Mitchell and Griffiths (1980), and Lapidus and Pinder (1982). The
following introduction is a summary of the one presented in the textbook of Thomas (1995).

Consider the model partial differential equation

\[
u_t = \mu(x, t)u_x + \nu(x, t)u_{xx}
\]  

(C.3)

defined on the spatial and temporal domains

\( \mathcal{R}_x = [x_0, x_n] \) and \( \mathcal{T}_t = [t_0, t_n] \).

To construct a basic finite-difference numerical scheme the computational domain is first dis-
cretised into a number of equidistant grid points

\[
x_i = i \Delta x + x_0, \quad \text{for } i = 0, 1, \ldots, n_x
\]

\[
t^j = s \Delta t + t_0, \quad \text{for } j = 0, 1, \ldots, n_t.
\]

The well-known definition of a derivative

\[
f'(x) = \lim_{x \to 0} \frac{f(x + h) - f(x)}{h}
\]

suggests the one-sided approximation

\[
u_x \approx \frac{u_{i+1}^s - u_i^s}{\Delta x} \quad (C.4)
\]
for the first-order spatial derivative. Performing a Taylor expansion

\[ u_{i+1}^s = u ((i + 1) \Delta x, s \Delta t) = u (i \Delta x, s \Delta t) + \frac{\partial u}{\partial x} (i \Delta x, s \Delta t) \frac{\Delta x}{1!} + \frac{\partial^2 u}{\partial x^2} (i \Delta x, s \Delta t) \frac{\Delta x^2}{2!} + \cdots \]

and rearranging the variables to obtain

\[ \frac{u_{i+1}^s - u_i^s}{\Delta x} = \frac{\partial u}{\partial x} + O(\Delta x) \]

shows that the approximation has an error of the order \( O(\Delta x) \). It can be shown in a similar fashion that the spatially-centred difference approximations

\[ u_x \approx \frac{u_{i+1}^s - u_i^s - u_{i-1}^s}{2\Delta x} \]

(C.5)

and

\[ u_{xx} \approx \frac{u_{i+1}^s - 2u_i^s + u_{i-1}^s}{\Delta x^2} \]

(C.6)

are both accurate to second order, \( O(\Delta x^2) \).

For the time derivative, the one-sided approximation

\[ u_t = \frac{u_{i+1}^s - u_i^s}{\Delta t} \]

(C.7)

is often preferred, where the unknown solutions at the time step \( s + 1 \) are calculated using the known solutions at the present time \( s \). Even though the approximation is only \( O(\Delta t) \) accurate, it is possible to construct numerical schemes using (C.7) that are \( O(\Delta t^2) \) accurate.

A numerical scheme where the unknown values \( u_{i+1}^s \) are calculated using only the solutions \( u_i^s \) is referred to as an explicit scheme. By contrast, some schemes require \( u_{i+1}^s \) to be expressed as a function of \( u_i^s \) as well as the remaining \( u_{k+1}^s \). These methods are referred to as implicit schemes.

For the rest of this chapter, the operator notation

\[ \delta_x u_i = \frac{u_{i+1}^s - u_i^s}{2\Delta x} \]

\[ \delta_x^2 u_i = \frac{u_{i+1}^s - 2u_i^s + u_{i-1}^s}{\Delta x^2} \]

will be used.

C.2.2 Stability

An important issue in numerical schemes is that of stability. Loosely defined, a numerical scheme is said to be stable if errors introduced during computation do not grow exponentially with every time step (Thomas, 1995). Alternatively stated, a scheme is stable if the computational errors can be made arbitrarily small (Lapidus and Pinder, 1982). Numerical schemes with a restriction on the choice of grid sizes \( \Delta x \) and \( \Delta t \) are referred to as being conditionally stable, whereas schemes not subjected to such a restriction are unconditionally stable (Lapidus and Pinder, 1982). Although this is not always true, explicit schemes tend to fall in the former category, and implicit schemes in the latter. For a mathematical treatment of stability, the extensive body of literature can be consulted (see, e.g., Mitchell and Griffiths, 1980; Lapidus and Pinder, 1982; Thomas, 1995).
C.2.3 Boundary conditions

To uniquely solve a partial differential equation, it is generally necessary to specify a combination of initial

\[ u(t_0, x), \quad x \in \overline{R}_x \]

and boundary conditions

\[ u(t, \partial R_x), \quad t > 0, \]

where \( t_0 \) refers to the initial time and \( \partial R_x \) to the boundaries \( u(t, x_0) \) and \( u(t, x_n) \). It is possible to distinguish between (see, e.g., Lapidus and Pinder, 1982)

- **Pure initial value** problems: the solutions are specified at \( t_0 \) and on one of the boundaries, e.g., \( u(t, x_0) \);
- **Initial-boundary value** problems: the solutions are specified at \( t_0 \) and on \( \partial R_x \). It is important to note that parabolic schemes fall in this category;
- **Pure boundary value** problems: the solutions are specified on \( \partial R_i \) and \( \partial R_x \).

The following four possibilities are included among the types of boundary conditions (see, e.g., Lapidus and Pinder, 1982):

- The **Dirichlet** condition: the solution is specified at the boundary;
- The **Neumann** condition: the slope is specified at the boundary;
- The **Cauchy** condition: both the solution and slope are specified on the boundary using two separate equations;
- The **Robbins** condition: the solution and slope are specified on the boundary using a single first-order differential equation.

C.3 One-dimensional parabolic schemes

C.3.1 The forward-difference explicit scheme

One of the first finite-difference schemes derived in, e.g., Lapidus and Pinder (1982) is the **Classic Explicit Approximation**. Using a one-sided approximation for time and a centred approximation for the spatial variable at time \( s \), the numerical equivalent of (C.3) is given by

\[ \frac{u_i^{s+1} - u_i^s}{\Delta t} = (\mu^s \delta_x + \nu^s \delta_x^2) u_i^s. \]  

(C.8)

A stability analysis shows that the method is stable when the condition

\[ \frac{\Delta t}{\Delta x^2} \leq \frac{1}{2} \]

is satisfied. As a result of the chosen approximations, the method is \( O(\Delta t, \Delta x^2) \) accurate.
C.3.2 The backward-difference implicit scheme

A second, simple finite-difference scheme derived in, e.g., Lapidus and Pinder (1982) uses a centred approximation for the spatial variable at time $s+1$ is used, resulting in the numerical scheme

$$\frac{u_{i}^{s+1} - u_{i}^{s}}{\Delta t} = (\mu_{i}^{s+1} \delta_{x} + \nu_{i}^{s+1} \delta_{x}^2) u_{i}^{s+1}. \quad (C.9)$$

This leads to $n_x-1$ coupled equations with $n_x+1$ unknown variables. The boundary conditions on $\partial R_x$ reduce the number of unknown variables to $n_x - 1$, and the system can be solved uniquely for a given initial condition.

It is possible to express (C.9) in matrix notation

$$A u^{s+1} = d,$$

where $A$ is the coefficient matrix and $d$ a vector consisting of the known solutions $u_{i}^{s}$, as well as the boundary values $u_{0}^{s+1}$ and $u_{n_x}^{s+1}$. The inclusion of the boundary values in $d$ leads to the removal of the entries $A_{0,0}$ and $A_{n_x,n_x}$ from the coefficient matrix, thereby reducing $A$ to a tri-diagonal form. Consequently

$$u^{s+1} = A^{-1} d$$

can be solved using the relatively simple and computationally effective Thomas algorithm (see Section C.5).

Although the implicit method is more computationally intensive compared to the forward-difference explicit method, it has the advantage of being unconditionally stable, while the choice of approximations again leads to a method that is $O(\Delta t, \Delta x^2)$ accurate.

C.3.3 The Crank-Nicolson implicit scheme

Crank and Nicolson (1947) showed that the accuracy in the time direction can be improved by replacing the centred spatial approximation with a time average between times $s$ and $s + 1$:

$$\frac{u_{i}^{s+1} - u_{i}^{s}}{\Delta t} = \frac{\mu}{2} \delta_{x} (u_{i}^{s+1} + u_{i}^{s}) + \frac{\nu}{2} \delta_{x}^2 (u_{i}^{s+1} + u_{i}^{s}). \quad (C.10)$$

The result is a method that is unconditionally stable and $O(\Delta t^2, \Delta x^2)$ accurate for constant coefficients $\mu$ and $\nu$, even though a one-sided approximation is used for time. To maintain unconditional stability and $O(\Delta t^2, \Delta x^2)$ accuracy, variable coefficients should be computed at the intermediate time $t^{s+1/2}$ (see, e.g., Tadjeran, 2007)

$$\frac{u_{i}^{s+1} - u_{i}^{s}}{\Delta t} = \frac{1}{2^{\mu_{i}^{s+1/2} \delta_{x}} (u_{i}^{s+1} + u_{i}^{s}) + \frac{1}{2^{\nu_{i}^{s+1/2} \delta_{x}^2}} (u_{i}^{s+1} + u_{i}^{s}). \quad (C.11)$$

As discussed in the textbook of Lapidus and Pinder (1982), the Crank-Nicolson scheme can be easily extended to deal with general, quasilinear parabolic partial differential equations

$$u_t = \psi (u, x, t, u_x, u_{xx}), \quad (C.12)$$
approximated by
\[
\frac{u^{s+1}_i - u^s_i}{\Delta t} = \psi \left[ \frac{1}{2} u^{s+1}_i + u^s_i, x_i, t^{s+1/2}, \frac{1}{2} \delta_x (u^{s+1}_i + u^s_i), \frac{1}{2} \delta_x^2 (u^{s+1}_i + u^s_i) \right]
\]
with $O(\Delta t^2, \Delta x^2)$ accuracy.

### C.3.4 Boundary conditions in one dimension

- **The Dirichlet condition**
  \[
u(x_0, t) = g(t),\]
  with $g(t)$ a known function, is implemented in the numerical scheme in a straightforward manner,
  \[
u_0^s = g^s.
\]

- **The Neumann condition**
  \[
u_x(x_0, t) = g(t)
\]
can be approximated using the one-sided discretisation
  \[
  \frac{u^s_i - u^s_0}{\Delta x} = g^s.
\]
  If a specific numerical scheme was chosen for its $O(\Delta x^2)$ accuracy, the one-sided approximation can lead to results that are only $O(\Delta x)$ accurate (see, e.g., Thomas, 1995). To ensure second-order accuracy, the centred approximation
  \[
  \frac{u^s_i - u^s_{-1}}{2\Delta x} = g^s
\]
should rather be used, at the expense of introducing a new grid point at $x_{-1}$. Extending $R_x$ to include the new grid point, (C.16) can be used to eliminate $u_{-1}$ in favour of $u_1$.

- A third possible type of boundary condition that can be imposed on (C.3) is of the form
  \[
u(x_0, t) + \nu_x(x_0, t) = g(t).
\]
The first-order numerical approximation for the Robbins condition (C.17) is given by
  \[
  u_0^s + \frac{u^s_i - u^s_0}{\Delta x} = g^s,
\]
and the second-order approximation by
  \[
  u_0^s + \frac{u^s_i - u^s_{-1}}{2\Delta x} = g^s.
\]
C.4 Two-dimensional parabolic schemes

To illustrate the implementation of two-dimensional numerical methods, the partial differential equation

\[ u_t = u_{xx} + u_{yy} \tag{C.19} \]

will serve as the model equation. The definition of the operator notation for the derivatives introduced in the previous section is modified accordingly to include the added dimension:

\[ \delta^2_x u_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} \]

and

\[ \delta^2_y u_{i,j} = \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta y^2} . \]

As a logical extension of the one-dimensional Crank-Nicolson scheme, e.g., Lapidus and Pinder (1982) state that one might choose the approximation

\[ \frac{u^{s+1}_{i,j} - u^s_{i,j}}{\Delta t} = \frac{1}{2} \delta^2_x \left( u^{s+1/2}_{i,j} + u^s_{i,j} \right) + \frac{1}{2} \delta^2_y \left( u^{s+1/2}_{i,j} + u^s_{i,j} \right), \]

or, in simplified form,

\[ \left( 1 - \frac{\Delta t}{2} \delta^2_x - \frac{\Delta t}{2} \delta^2_y \right) u^{s+1}_{i,j} = \left( 1 + \frac{\Delta t}{2} \delta^2_x + \frac{\Delta t}{2} \delta^2_y \right) u^s_{i,j}. \tag{C.20} \]

Although unconditionally stable and \( O(\Delta t^2, \Delta x^2, \Delta y^2) \) accurate, the resulting coefficient matrix \( A \) is penta-diagonal. To solve the unknown functions would require the use of Gauss elimination or an iterative process (e.g., Gauss-Seidel, Jacobi, ...), all of which are computationally expensive for higher-dimensional problems.

A number of alternative methods have been developed that preserve the tri-diagonal nature of \( A \). The basic idea behind these methods is to split the numerical scheme into a two-tiered set of equations. In the first tier, the numerical scheme solves the unknown values at an intermediate time step \( s + 1/2 \). The newly acquired solutions are then used to solve the partial differential equation at the time step \( s + 1 \).

C.4.1 The Alternating Direction Implicit scheme

*Alternating Direction Implicit* (ADI) schemes are listed among the two-dimensional numerical methods, and were first introduced by Peaceman and Rachford (1955). These authors showed that a practical scheme can be constructed by choosing one variable to be implicit (Section C.3.2) and the other to be explicit (Section C.3.1) for the first half of the time step:

\[ \frac{u^{s+1/2}_{i,j} - u^s_{i,j}}{\Delta t/2} = \delta^2_x u^{s+1/2}_{i,j} + \delta^2_y u^s_{i,j}, \]
with a rearrangement of the variables leading to
\[
\left(1 - \frac{\Delta t}{2} \delta_x^2\right) u_{i,j}^{s+1/2} = \left(1 + \frac{\Delta t}{2} \delta_y^2\right) u_{i,j}^s.
\] (C.21a)

As the name of the method suggests, the choice of implicit/explicit variable is alternated for the next half of the time step:
\[
\frac{u_{i,j}^{s+1} - u_{i,j}^{s+1/2}}{\Delta t/2} = \delta_x^2 u_{i,j}^{s+1/2} + \delta_y^2 u_{i,j}^{s+1},
\]
which can be simplified as
\[
\left(1 - \frac{\Delta t}{2} \delta_y^2\right) u_{i,j}^{s+1} = \left(1 + \frac{\Delta t}{2} \delta_x^2\right) u_{i,j}^{s+1/2}.
\] (C.21b)

From (C.21a) and (C.21b) it is clear that both time steps lead to a coupled set of equations with a tri-diagonal coefficient matrix.

Multiplying the left-hand side of (C.21a) with the term \(1 + \Delta t/2 \delta_z^2\), and noting that the operators on the same side commute, leads to (see, e.g., Thomas, 1995)
\[
\left(1 - \frac{\Delta t}{2} \delta_x^2\right) \left(1 + \frac{\Delta t}{2} \delta_y^2\right) u_{i,j}^{s+1/2} = \left(1 + \frac{\Delta t}{2} \delta_x^2\right) \left(1 + \frac{\Delta t}{2} \delta_y^2\right) u_{i,j}^s.
\]

The solutions at the time step \(s + 1/2\) can now be eliminated from the scheme using (C.21b)
\[
\left(1 - \frac{\Delta t}{2} \delta_x^2\right) \left(1 - \frac{\Delta t}{2} \delta_y^2\right) u_{i,j}^{s+1} = \left(1 + \frac{\Delta t}{2} \delta_x^2\right) \left(1 + \frac{\Delta t}{2} \delta_y^2\right) u_{i,j}^s.
\] (C.22a)

\[
\left(1 - \frac{\Delta t}{2} \delta_x^2 - \frac{\Delta t}{2} \delta_y^2 + \frac{(\Delta t)^2}{4} \delta_x^2 \delta_y^2\right) u_{i,j}^{s+1} = \left(1 + \frac{\Delta t}{2} \delta_x^2 + \frac{\Delta t}{2} \delta_y^2 + \frac{(\Delta t)^2}{4} \delta_x^2 \delta_y^2\right) u_{i,j}^s.
\] (C.22b)

Apart from the factor \(\Delta t^2 \delta_x^2 \delta_y^2 / 4\), the Peaceman-Rachford scheme is identical to the two-dimensional Crank-Nicolson scheme (C.20). The additional term has an error of \(O(\Delta t^2, \Delta x^2, \Delta y^2)\), implying an \(O(\Delta t^2, \Delta x^2, \Delta y^2)\) accuracy for the scheme as a whole. Moreover, the scheme is unconditionally stable for constant coefficients (see, e.g., Thomas, 1995).

As hinted at in a previous paragraph, the Peaceman-Rachford scheme is not the only available ADI method. It is possible to replace the simple form of the implicit approximation with a Crank-Nicolson approach, introduced by Douglas (1962):
\[
\frac{u_{i,j,s+1}^{t} - u_{i,j}^{t}}{\Delta t} = \frac{1}{2} \delta_x^2 \left(u_{i,j,s+1}^{t} + u_{i,j}^{t}\right) + \delta_y^2 u_{i,j}^{t}
\]
\[
\left(1 - \frac{\Delta t}{2} \delta_x^2\right) u_{i,j}^{t+1} = \left(1 + \frac{\Delta t}{2} \delta_x^2 + \Delta t \delta_y^2\right) u_{i,j}^{t}.
\] (C.23a)

and
\[
\frac{u_{i,j}^{t+1} - u_{i,j}^{t}}{\Delta t} = \frac{1}{2} \delta_x^2 \left(u_{i,j,s+1}^{t+1} + u_{i,j}^{t+1}\right) + \frac{1}{2} \delta_y^2 \left(u_{i,j}^{t+1} + u_{i,j}^{t}\right)
\]
\[
\left(1 - \frac{\Delta t}{2} \delta_y^2\right) u_{i,j}^{t+1} = \left(1 + \frac{\Delta t}{2} \delta_x^2 + \frac{\Delta t}{2} \delta_y^2\right) u_{i,j}^{t}.
\] (C.23b)
Note that an intermediate time step \( s + 1/2 \) is not involved in the discretisation. Subtracting (C.23a) from (C.23b) leads to the equation (Douglas, 1962)

\[
\left(1 - \frac{\Delta t}{2} \delta_x^2 \right) u_{i,j}^{s+1} = u_{i,j,s+1} - \frac{\Delta t}{2} \delta_y^2 u_{i,j}^s,
\]

(C.23c)

effectively replacing (C.23b) in the numerical scheme. Using the above equation to eliminate \( u_{i,j,s+1}^* \) from (C.23a) leads to

\[
\left(1 - \frac{\Delta t}{2} \delta_x^2 \right) \left(1 - \frac{\Delta t}{2} \delta_y^2 \right) u_{i,j}^{s+1} = \left(1 + \frac{\Delta t}{2} \delta_x^2 \right) \left(1 + \frac{\Delta t}{2} \delta_y^2 \right) u_{i,j}^s,
\]

(C.24)

a result that is identical to the one obtained from the Peaceman-Rachford splitting. The scheme is therefore also \( O(\Delta t^2, \Delta x^2, \Delta y^2) \) accurate, as well as unconditionally stable (see, e.g., Lapidus and Pinder, 1982). A number of additional splitting schemes can be found in the literature (see, e.g., Lapidus and Pinder, 1982; Thomas, 1995). For the present study, the Douglas scheme is chosen to solve the multi-dimensional transport equations (B.14) and (B.15).

Quasi-linear equations

\[
u_t = u_{xx} + u_{yy} + \psi(x, y, t, u)
\]

(C.25)

can be discretised in the Douglas scheme as

\[
\left(1 - \frac{\Delta t}{2} \delta_x^2 \right) u_{i,j,s+1}^* = \left(1 + \frac{\Delta t}{2} \delta_x^2 + \Delta t \delta_y^2 \right) u_{i,j}^s + \Delta t \psi \left(x_i, y_j, t^{s+1/2}, u_{i,j}^s \right).
\]

(C.26)

However, the above equation used with (C.23c) reduces the accuracy in the time direction (Douglas, 1962). The accuracy can be improved from \( O(\Delta t) \) to \( O(\Delta t^2) \) by first solving (C.26) and (C.23c) with \( \Delta t \) replaced by \( \Delta t/2 \), leading to an intermediate estimate \( \hat{u}_{i,j}^{s+1/2} \). In the second step, (C.26) and (C.23c) are solved using \( \Delta t \) and \( \psi \) replaced by (Douglas, 1962)

\[
\hat{\psi} \left(x_i, y_j, t^{s+1/2}, \hat{u}_{i,j}^{s+1/2} \right).
\]

The \( O(\Delta t^2, \Delta x^2, \Delta y^2) \) accuracy is again obtained, at the expense of doubling the number of equations to be solved (Douglas, 1962).

C.4.2 Boundary conditions in two dimensions

It was mentioned in Section C.3.4 that a seemingly innocuous choice of boundary condition can easily lead to a reduction in the accuracy of a numerical scheme. For two-dimensional schemes additional care should be taken when specifying the boundary conditions at the intermediate time step. The numerical solutions \( u_{i,j}^{s+1/2} \) are not necessarily an approximation to the actual solutions at a given time value (Mitchell and Griffiths, 1980), and therefore the boundary condition at \( s + 1 \) does not always directly translate into a condition for \( s + 1/2 \). To maintain accuracy in the method, the intermediate boundary values should be expressed, if possible, as functions of the boundary values at \( s \) and \( s + 1 \) (Mitchell and Griffiths, 1980).
Dirichlet boundary condition

Consider the model equation (C.19), subject to the Dirichlet boundary condition

\[ u(0, y, t) = g(y, t), \quad \text{for } t > 0 \]  

(C.27)

with the numerical equivalent

\[ u_{0,j}^{s+1} = g_j^{s+1}. \]  

(C.28)

For the Peaceman-Rachford ADI scheme, it can be shown that (see, e.g., Mitchell and Griffiths, 1980)

\[ u_{i,j}^{s+1/2} = \frac{1}{2} \left( 1 - \frac{\Delta t}{2} \delta^2_y \right) u_{i,j}^{s+1} + \frac{1}{2} \left( 1 + \frac{\Delta t}{2} \delta^2_y \right) u_{i,j}^s. \]  

(C.29)

Substituting the values \( u_{i,j}^{s+1} \) and \( u_{i,j}^s \) using (C.28) leads to the correct form of the boundary condition

\[ u_{0,j}^{s+1/2} = \frac{1}{2} \left( 1 - \frac{\Delta t}{2} \delta^2_y \right) g_{j}^{s+1} + \frac{1}{2} \left( 1 + \frac{\Delta t}{2} \delta^2_y \right) g_{j}^s. \]  

(C.30)

The condition for the Douglas ADI scheme follows directly from (C.23c)

\[ u_{0,j,s}^{s+1} = g_{j}^{s+1} - \frac{\Delta t}{2} \delta^2_y \left( g_{j}^{s+1} - g_{j}^s \right). \]  

(C.31)

If (C.28) is time-independent, the intermediate condition reduces to

\[ u_{0,j}^{s+1/2} = g_{j} \]  

(C.32)

for both the Peaceman-Rachford and Douglas schemes. If the initial condition is time-dependent, but not a function of \( y \), (C.28) again reduces to (C.32).

Neumann boundary condition

Consider the model equation (C.19), subject to the Neumann boundary condition

\[ u_x(0, y, t) = g(y, t), \quad \text{for } t > 0. \]  

(C.33)

From the second-order approximation of the Neumann boundary condition it follows that

\[ u_{i-1,j}^{s+1} - u_{i,j}^{s+1} = -2 \Delta x g_j^{s+1}. \]  

(C.34)

Using (C.29), e.g., Thomas (1995) shows that the solutions at the intermediate time step for \( i = -1 \) and \( i = 1 \) can be written as

\[ u_{-1,j}^{s+1/2} = \frac{1}{2} \left( 1 - \frac{\Delta t}{2} \delta^2_y \right) u_{-1,j}^{s+1} + \frac{1}{2} \left( 1 + \frac{\Delta t}{2} \delta^2_y \right) u_{-1,j}^s. \]  

(C.35a)

and

\[ u_{1,j}^{s+1/2} = \frac{1}{2} \left( 1 - \frac{\Delta t}{2} \delta^2_y \right) u_{1,j}^{s+1} + \frac{1}{2} \left( 1 + \frac{\Delta t}{2} \delta^2_y \right) u_{1,j}^s. \]  

(C.35b)
Subtracting (C.35b) from (C.35a), and using (C.34) to eliminate the solutions at \( s + 1 \) leads to the intermediate Neumann boundary condition (Thomas, 1995)

\[
\frac{u_{s+1/2}}{u_{1,j}} - \Delta x \left( 1 - \frac{\Delta t}{2} \frac{\delta^2}{\delta_y^2} \right) g_j^{s+1} + \frac{1}{2} \left( 1 + \frac{\Delta t}{2} \frac{\delta^2}{\delta_y^2} \right) (u^s_{1,j} - u^s_{1,j}) .
\] (C.36)

As (C.34) holds for all values of time, except possibly at \( s = 0 \), the boundary conditions can be reduced to

\[
\frac{u_{s+1/2}}{u_{1,j}} - \Delta x \left( 1 - \frac{\Delta t}{2} \frac{\delta^2}{\delta_y^2} \right) g_j^{s+1} - \Delta x \left( 1 + \frac{\Delta t}{2} \frac{\delta^2}{\delta_y^2} \right) g_j^s
\] (C.37)

for \( s > 0 \).

Following the same line of reasoning, (C.23c) leads to the boundary condition

\[
u^*_{s,j,s+1} = u^*_{s,j,s+1} - 2\Delta x \left( 1 - \frac{\Delta t}{2} \frac{\delta^2}{\delta_y^2} \right) g_j^{s+1} + \frac{\Delta t}{2} \frac{\delta^2}{\delta_y^2} (u^s_{1,j} - u^s_{1,j})
\] (C.38)

for the Douglas ADI scheme. If the gradient at the boundary is zero, the conditions (C.37) and (C.38) reduce to the simple form

\[
u_{s+1/2}^{s+1} = u_{1,j}^{s+1/2}.
\] (C.39)

**Robbins boundary condition**

It follows from the derivation presented in Section 5.2.2 that a central source system requires a Robbins boundary condition, which can be stated in general terms as

\[
a(y)u(0, y, t) + b(y)u_x(0, y, t) = g(y),
\] (C.40)

Here \( a(y) \) and \( b(y) \) are coefficients determined by the physics of the problem studied. Unfortunately, deriving an intermediate boundary condition for (C.40) leads to new complications, as will be illustrated using the Douglas scheme.

With a slight re-arrangement of variables, the first and second-order approximations to (C.40) can respectively be written as

\[
u^0_{s+1} = \xi u^s_{1,j} + \frac{\Delta x}{b_j} g_j^{s+1}
\] (C.41a)

and

\[
u^{-1}_{s+1} = \frac{2a_j}{b_j} \Delta x u^s_0 + u^s_{1,j} - \frac{2\Delta x}{b_j} g_j^{s+1},
\] (C.41b)

where

\[
\xi = \left( 1 + \frac{a_j \Delta x}{b_j} \right)^{-1}.
\]

Using (C.31), the intermediate Robbins boundary condition for the Douglas scheme is derived from (C.41a) as

\[
u^0_{0,j,s+1} = \xi \left( 1 - \frac{\Delta t}{2} \frac{\delta^2}{\delta_y^2} \right) \left( u^s_{1,j} + \frac{\Delta x}{b_j} g_j^{s+1} \right) + \frac{\xi \Delta t}{2} \frac{\delta^2}{\delta_y^2} \left( u^s_{1,j} + \frac{\Delta x}{b_j} g_j^s \right),
\] (C.42a)
and from (C.41b) as
\[ u^*_{-1,j,s+1} = u^*_{1,j,s+1} + \frac{2\Delta x}{b_j} \left( 1 - \frac{\Delta t}{2} \delta_y^2 \right) \left( a_j u^*_{0,j} - g^*_j + 1 \right) + \frac{\Delta x \Delta t}{b_j} \delta_y^2 \left( a_j u^*_{0,j} - g^*_j \right). \] (C.42b)

Although formally correct, the proposed intermediate boundary conditions require the yet unknown values \( u^*_{0,j} \), and it is therefore necessary to find an alternative expression for the intermediate boundary condition. Fortunately, as shown in Section 5.3.1, is it possible to maintain numerical accuracy for the two-dimensional systems studied in Chapters 5 and 6 without constructing an intermediate boundary condition.

C.5 The Thomas algorithm

The one and two-dimensional numerical methods introduced in this chapter both rely on the solution of a tri-diagonal matrix. For this purpose, the very effective Thomas algorithm has been developed, and is discussed in most textbooks dealing with finite-difference methods, such as those of Mitchell and Griffiths (1980), Lapidus and Pinder (1982), and Thomas (1995).

Consider the set of coupled equations
\[
\begin{align*}
A_0 u_0 + B_1 u_1 + C_2 u_2 &= d_1 \\
A_1 u_1 + B_2 u_2 + C_3 u_3 &= d_2 \\
&\vdots \\
A_{m-3} u_{m-3} + B_{m-2} u_{m-2} + C_{m-1} u_{m-1} &= d_{m-2} \\
A_{m-2} u_{m-2} + B_{m-1} u_{m-1} + C_m u_m &= d_{m-1},
\end{align*}
\] (C.43)

with known coefficients \( A_i, B_i, C_i \), and known values \( d_i \). Additionally, (C.43) is subjected to the "boundary conditions"
\[
\begin{align*}
u_0 &= v_1 u_1 + v_2 u_2 + v_3 \\
u_m &= v_4 u_{m-1} + v_5 u_{m-2} + v_6,
\end{align*}
\] (C.44)

where the various \( v_i \) are also known. Using the boundary conditions to eliminate \( u_0 \) and \( u_m \) from (C.43), the coupled set of equations can be expressed in the matrix form
\[
Au = d,
\] (C.45)

where
\[
A = \begin{bmatrix}
B_1 & C_2 \\
A_1 & B_2 & C_3 \\
A_2 & B_3 & C_4 \\
& \cdots & \cdots \\
A_{m-3} & B_{m-2} & C_{m-1} \\
A_{m-2} & B_{m-1}
\end{bmatrix}
\]
is the coefficient matrix with modified elements
\[
B_1 \equiv B_1 + A_0 v_1 \\
C_2 \equiv C_2 + A_0 v_2 \\
A_{m-2} \equiv A_{m-2} + C_m v_5 \\
B_{m-1} \equiv B_{m-1} + C_m v_4,
\]

\(u\) is the vector containing the unknown quantities
\[
u = \begin{bmatrix}
    u_1 \\
    u_2 \\
    u_3 \\
    \vdots \\
    u_{m-2} \\
    u_{m-1}
\end{bmatrix},
\]

and \(d\) is the vector containing the known quantities
\[
d = \begin{bmatrix}
    d_1 \\
    d_2 \\
    d_3 \\
    \vdots \\
    d_{m-2} \\
    d_{m-1}
\end{bmatrix},
\]

with redefined elements
\[
d_1 \equiv d_1 - A_0 v_3 \\
d_{m-1} \equiv d_{m-1} - C_m v_6.
\]

While most introductory texts on finite-difference methods present a limited Thomas algorithm valid only for the boundary conditions \(u_0 = v_3\) and \(u_m = v_6\), Steenkamp (1995) showed that it is possible to incorporate the more general boundary conditions (C.44) into a modified algorithm:
\[
Z_i = B_i - c'_{i-1} A_{i-1}, \quad \text{for } i = 1, \ldots, m - 1 \\
c'_i = \frac{C_{i+1} - A_0 c'_{i-1}}{Z_i}, \quad \text{for } i = 1, \ldots, m - 1 \\
d'_i = \frac{d_i - d'_{i-1} A_{i-1}}{Z_i}, \quad \text{for } i = 1, \ldots, m - 1, \quad \text{(C.46)}
\]

where
\[
c'_0 = -v_1 \\
c'_{-1} = -v_2 \\
c'_{-i} = 0, \quad \text{for } i > 1 \\
d'_0 = v_3.
\]
With the exception of
\[ u_{m-1} = \frac{d'_{n-1} - c'_{n-1} (v_6 + d''_{m-2} v_5)}{1 + c'_{m-1} (v_4 - c''_{m-2} v_5)}, \] (C.47)
the vector \( u \) is solved recursively using the expression
\[ u_i = d'_i - c'_i u_{i+1}, \quad \text{for} \quad i = m - 2, m - 3, \ldots, 2, 1. \] (C.48)

### C.6 Numerical schemes for the transport equation

#### C.6.1 Spherically-symmetric steady-state scheme

The numerical schemes introduced in the previous section can be advanced by either stepping forward or backward in time. The only limitation is that the stepping direction has to remain fixed for a given problem. To construct a numerical scheme for the steady-state transport equation, a new stepping parameter has to be chosen, with the logical choice being the momentum \( p \). The limitation on the stepping direction implies that it is not possible to include both momentum losses and gains in the numerical scheme, as this would make it necessary to step forward and backward in \( p \).

The time-independent version of the spherically symmetric transport equation (B.15) used in Chapter 5
\[ a_{rr} f_{rr} + a_r f_r + a_p f_p + a_f f + Q = 0 \] (C.49)
includes only energy losses, and it is therefore more convenient to step backward in \( p \). The discretisation of the transport equation is done using the Crank-Nicolson scheme introduced in Section C.3.3,
\[ \frac{a_{rr}}{2} \delta_r^2 (f_i^{s+1} + f_i^s) + \frac{a_r}{2} \delta_r (f_i^{s+1} + f_i^s) - \frac{a_p}{\Delta \ln p} (f_i^{s+1} + f_i^s) + \frac{a_f}{2} (f_i^{s+1} + f_i^s) + Q_i^{s+1/2} = 0. \] (C.50a)

The above equation can be expanded to obtain
\[ \frac{a_{rr}}{2 \Delta r^2} (f_{i+1}^{s+1} - f_i^{s+1} + f_{i-1}^{s+1}) + \frac{a_r}{2 \Delta r^2} (f_{i+1}^{s+1} - 2 f_i^{s+1} + f_{i-1}^{s+1}) + \frac{a_r}{4 \Delta r} (f_{i+1}^{s+1} - f_{i-1}^{s+1}) + \frac{a_p}{4 \Delta r} (f_{i+1}^{s} - f_{i-1}^{s}) - \frac{a_p}{\Delta \ln p} (f_i^{s+1} - f_i^s) + \frac{a_f}{2} (f_i^{s+1} + f_i^s) + Q_i^{s+1/2} = 0. \] (C.50b)

The minus sign appearing in \(-\Delta \ln p\) is necessary when stepping backward in \( p \). Rearranging the terms according to the time index leads to the tri-diagonal set of coupled equations
\[ (z_{rr} - z_r) f_{i-1}^{s+1} + (2 z_{rr} + z_p - z_f) f_i^{s+1} + (z_{rr} + z_r) f_{i+1}^{s+1} = \]
\[ - (z_{rr} - z_r) f_{i-1}^s + (2 z_{rr} - z_p - z_f) f_i^s - (z_{rr} + z_r) f_{i+1}^s + Q_i^{s+1/2}. \] (C.51)
A comparison with the spherically-symmetric transport equation (B.15) shows that

\[ z_{rr} = \frac{1}{2\Delta r^2} \kappa_{rr}, \]
\[ z_r = \frac{1}{4\Delta r} \left( \frac{\partial \kappa_{rr}}{\partial r} + \frac{2\kappa_{rr}}{r} - V_r \right), \]
\[ z_p = \frac{1}{\Delta \ln p} \left( \frac{2V_r}{3r} + \frac{1}{3} \frac{\partial V_r}{\partial r} + k_p B^2 p \right), \]
\[ z_f = 2k_p B^2 p. \]

All position-dependent coefficients are evaluated at the radial position \( i \), while momentum-dependent coefficients are evaluated at the \( s + 1/2 \) momentum step.

### C.6.2 One-dimensional time-dependent scheme

With the added dimension of time, the spherically-symmetric, time-dependent transport equation (B.15) used in Chapter 5

\[ f_t = a_{rr} f_{rr} + a_{pp} f_{pp} + a_r f_r + a_p f_p + a_f f + Q \]  \hspace{1cm} (C.52)

is discretised using the Douglas scheme introduced in Section C.4.1. This leads to the equations

\[ \frac{f^{s+1}_{i,j} - f^s_{i,j}}{\Delta t} = a_{rr} \frac{\delta^2}{2} \left( f^{s+1}_{i,j} + f^s_{i,j} \right) + a_r \frac{\delta_r}{2} \left( f^{s+1}_{i,j} + f^s_{i,j} \right) + a_p \frac{\delta_p}{2} \left( f^{s+1}_{i,j} + f^s_{i,j} \right) + a_f \frac{1}{2} \left( f^{s+1}_{i,j} + f^s_{i,j} \right) + Q^{s+1/2}_{i,j} \]  \hspace{1cm} (C.53a)

and

\[ \frac{f^s_{i,j} - f^{s-1}_{i,j}}{\Delta t} = a_{rr} \frac{\delta^2}{2} \left( f^s_{i,j} + f^{s-1}_{i,j} \right) + a_r \frac{\delta_r}{2} \left( f^s_{i,j} + f^{s-1}_{i,j} \right) + a_p \frac{\delta_p}{2} \left( f^s_{i,j} + f^{s-1}_{i,j} \right) + a_f \frac{1}{2} \left( f^s_{i,j} + f^{s-1}_{i,j} \right) + Q^{s+1/2}_{i,j}. \]  \hspace{1cm} (C.53b)

The above equations can be expanded as

\[ \frac{f^s_{i,j} - f^{s-1}_{i,j}}{\Delta t} = a_{rr} \frac{\delta^2}{2} \left( f^s_{i+1,j} - 2f^s_{i,j} + f^s_{i-1,j} \right) + a_r \frac{\delta_r}{2} \left( f^s_{i+1,j} - 2f^s_{i,j} + f^s_{i-1,j} \right) + a_p \frac{\delta_p}{2} \left( f^s_{i+1,j} - 2f^s_{i,j} + f^s_{i-1,j} \right) + a_f \frac{1}{2} \left( f^s_{i,j} + f^{s-1}_{i,j} \right) + Q^{s+1/2}_{i,j}, \]  \hspace{1cm} (C.54a)
and

\[
\frac{f_{i,j}^{s+1} - f_{i,j}^s}{\Delta t} = \frac{a_{rr}}{2\Delta r^2} \left( f_{i+1,j}^s - 2f_{i,j}^s + f_{i-1,j}^s \right) + \frac{a_{rr}}{2\Delta r^2} \left( f_{i+1,j}^s - 2f_{i,j}^s + f_{i-1,j}^s \right) + \frac{a_r}{4\Delta r} \left( f_{i+1,j}^s - f_{i-1,j}^s \right) + \frac{a_{pp}}{2\Delta (\ln p)^2} \left( f_{i,j+1}^s - 2f_{i,j}^s + f_{i,j-1}^s \right) + \frac{a_{pp}}{2\Delta (\ln p)^2} \left( f_{i,j+1}^s - 2f_{i,j}^s + f_{i,j-1}^s \right) + \frac{a_p}{4\Delta \ln p} \left( f_{i,j+1}^s - f_{i,j-1}^s \right) + \frac{a_p}{4\Delta \ln p} \left( f_{i,j+1}^s - f_{i,j-1}^s \right) + \frac{a_f}{2} \left( f_{i,j+1}^s + f_{i,j-1}^s \right) + Q_{i,j}^{s+1/2}.
\]

(C.55b)

Performing the usual subtraction, (C.54b)–(C.54a), and multiplying the result with a factor of two provides the alternative equation

\[
\frac{2}{\Delta t} \left( f_{i,j}^{s+1} - f_{i,j}^s \right) = \frac{a_{pp}}{\Delta \ln p^2} \left( f_{i,j+1}^{s+1} - 2f_{i,j}^{s+1} + f_{i,j-1}^{s+1} \right) - \frac{a_{pp}}{\Delta \ln p^2} \left( f_{i,j+1}^s - 2f_{i,j}^s + f_{i,j-1}^s \right) + \frac{a_p}{2\Delta \ln p} \left( f_{i,j+1}^s - f_{i,j-1}^s \right) - \frac{a_p}{2\Delta \ln p} \left( f_{i,j+1}^s - f_{i,j-1}^s \right) + a_f \left( f_{i,j+1}^s - f_{i,j}^s \right).
\]

(C.54c)

Re-arranging (C.54a) and (C.54c) according to indices leads to

\[
(-z_{rr} + z_r) f_{i-1,j}^s + (z_t + 2z_{rr} - z_f) f_{i,j}^s - (z_{rr} + z_r) f_{i+1,j}^s = (z_{rr} - z_r) f_{i+1,j}^s + (z_t - 2z_{rr} - 2z_{pp} + z_f) f_{i,j}^s + (z_{rr} + z_r) f_{i+1,j}^s + (z_{pp} + z_p) f_{i,j+1}^s + (z_{pp} + z_p) f_{i,j+1}^s + Q_{i,j}^{s+1/2}
\]

(C.55a)

and

\[
(-z_{pp} + z_p) f_{i,j+1}^{s+1} + 2(z_t + z_{pp} - z_f) f_{i,j}^{s+1} - (z_{pp} + z_p) f_{i,j+1}^{s+1} = (-z_{pp} + z_p) f_{i,j+1}^s + 2z_{pp} f_{i,j}^s + (z_{pp} + z_p) f_{i,j+1}^s + 2(z_t - z_f) f_{i,j}^s,
\]

(C.55b)

where

\[
\begin{align*}
    z_t &= \frac{1}{\Delta t} \\
    z_{rr} &= \frac{1}{2\Delta r^2} \kappa_{rr} \\
    z_r &= \frac{1}{4\Delta r} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \kappa_{rr}) - V_r \right] \\
    z_{pp} &= \frac{1}{\Delta \ln p^2} \kappa_{pp} \\
    z_p &= \frac{1}{2\Delta \ln p} \left[ \frac{1}{3r^2} \frac{\partial}{\partial r} (r^2 V_r) + k_p B^2 p + 3\kappa_{pp} \right] \\
    z_f &= 2k_p B^2 p.
\end{align*}
\]

(C.54a)
C.6.3 Two-dimensional steady-state scheme

The steady-state version of the axisymmetric transport equation (B.14) used in Chapter 6

\[ a_{rr} f_{rr} + a_{\theta\theta} f_{\theta\theta} + a_r f_r + a_\theta f_\theta + a_p f_p + a_f f + Q = 0 \]  
(C.56)

is also discretised with the Douglas scheme ADI method, resulting in the two sets of equations

\[
\begin{align*}
\frac{a_{rr}}{2} \delta_r^2 (f_{i,j}^s + f_{i,j}^s) + \frac{a_r}{2} \delta_r (f_{i,j}^s + f_{i,j}^s) \\
+ a_{\theta\theta} \delta_\theta^2 f_{i,j}^s + a_\theta \delta_\theta f_{i,j}^s \\
- \frac{a_p}{\Delta \ln p} (f_{i,j}^s - f_{i,j}^s) + \frac{a_f}{2} (f_{i,j}^s + f_{i,j}^s) + Q_{i,j}^{s+1/2} = 0
\end{align*}
\]  
(C.57a)

and

\[
\begin{align*}
\frac{a_{rr}}{2} \delta_r^2 (f_{i,j+1}^s + f_{i,j}^s) + \frac{a_r}{2} \delta_r (f_{i,j+1}^s + f_{i,j}^s) \\
+ \frac{a_{\theta\theta}}{2} \delta_\theta^2 (f_{i,j+1}^s + f_{i,j}^s) + \frac{a_\theta}{2} \delta_\theta (f_{i,j+1}^s + f_{i,j}^s) \\
- \frac{a_p}{\Delta \ln p} (f_{i,j+1}^s - f_{i,j}^s) + \frac{a_f}{2} (f_{i,j+1}^s + f_{i,j}^s) + Q_{i,j}^{s+1/2} = 0
\end{align*}
\]  
(C.57b)

or, in expanded form,

\[
\begin{align*}
\frac{a_{rr}}{2 \Delta r^2} (f_{i+1,j}^s - 2f_{i,j}^s + f_{i-1,j}^s) + \frac{a_r}{2 \Delta r^2} (f_{i+1,j}^s - 2f_{i,j}^s + f_{i-1,j}^s) \\
+ \frac{a_{\theta\theta}}{2 \Delta \theta^2} (f_{i,j+1}^s + f_{i,j}^s) + \frac{a_\theta}{2 \Delta \theta^2} (f_{i,j+1}^s + f_{i,j}^s) \\
- \frac{a_p}{\Delta \ln p} (f_{i,j}^s - f_{i,j}^s) + \frac{a_f}{2} (f_{i,j}^s + f_{i,j}^s) + Q_{i,j}^{s+1/2} = 0
\end{align*}
\]  
(C.58a)

and

\[
\begin{align*}
\frac{a_{rr}}{2 \Delta r^2} (f_{i+1,j}^s - 2f_{i,j}^s + f_{i-1,j}^s) + \frac{a_r}{2 \Delta r^2} (f_{i+1,j}^s - 2f_{i,j}^s + f_{i-1,j}^s) \\
+ \frac{a_{\theta\theta}}{2 \Delta \theta^2} (f_{i,j+1}^s - 2f_{i,j}^s + f_{i,j-1}^s) + \frac{a_\theta}{2 \Delta \theta^2} (f_{i,j+1}^s - 2f_{i,j}^s + f_{i,j-1}^s) \\
+ \frac{a_p}{\Delta \ln p} (f_{i,j}^s - f_{i,j}^s) + \frac{a_f}{2} (f_{i,j}^s + f_{i,j}^s) + Q_{i,j}^{s+1/2} = 0
\end{align*}
\]  
(C.58b)

Subtracting (C.58a) from (C.58b), and multiplying the result by a factor of two leads to the alternative equation

\[
\begin{align*}
\frac{a_{\theta\theta}}{\Delta \theta^2} (f_{i,j+1}^s - 2f_{i,j}^s + f_{i,j-1}^s) - \frac{a_{\theta\theta}}{\Delta \theta^2} (f_{i,j+1}^s - 2f_{i,j}^s + f_{i,j-1}^s) \\
+ \frac{a_\theta}{2 \Delta \theta} (f_{i,j+1}^s - f_{i,j-1}^s) - \frac{a_\theta}{2 \Delta \theta} (f_{i,j+1}^s - f_{i,j-1}^s) \\
- \frac{2a_p}{\Delta \ln p} (f_{i,j}^s - f_{i,j}^s) + a_f (f_{i,j}^s - f_{i,j}^s) = 0
\end{align*}
\]  
(C.58c)
that is used to replace (C.58b). Rearranging the variables in (C.58a) and (C.58c) according to the time and position indices leads to the tri-diagonal sets of equations

\[
(z_{rr} - z_r) f^*_{i-1,j} - (2z_{rr} + z_p - z_f) f^*_{i,j} + (z_{rr} + z_r) f^*_{i+1,j} = \\
- z_{rr} f^*_{i,j} + (2z_{rr} + 2z_{\theta\theta} - z_p - z_f) f^*_{i,j} - (z_{rr} + z_r) f^*_{i+1,j} \\
- (z_{\theta\theta} - z_\theta) f^*_{i,j-1} - (z_{\theta\theta} + z_\theta) f^*_{i,j+1} - Q^{*+1/2}_{i,j} \tag{C.59a}
\]

and

\[
(z_{\theta\theta} - z_\theta) f^*_{i,j+1} - 2 (z_{\theta\theta} + z_p - z_f) f^*_{i,j+1} + (z_{\theta\theta} + z_\theta) f^*_{i,j+1} = \\
(z_{\theta\theta} - z_\theta) f^*_{i,j-1} - 2 z_{\theta\theta} f^*_{i,j} + (z_{\theta\theta} + z_\theta) f^*_{i,j+1} - 2 (z_p - z_f) f^*_{i,j} \tag{C.59b}
\]

where a comparison with the axisymmetric transport equation (B.14) shows that the coefficients have the values

\[
\begin{align*}
z_{rr} &= \frac{1}{2 \Delta r^2} \kappa_{rr} \\
z_r &= \frac{1}{4 \Delta r} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \kappa_{rr} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \sin \theta \kappa_{\theta r} \right) - V_r \right] \\
z_{\theta\theta} &= \frac{1}{\Delta \theta^2} \kappa_{\theta\theta} \\
z_\theta &= \frac{1}{2 \Delta \theta} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r \kappa_{\theta r} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \sin \theta \kappa_{\theta \theta} \right) - \frac{V_\theta}{r} \right] \\
z_p &= \frac{1}{\Delta \ln p} \left[ \frac{1}{3r^2} \frac{\partial}{\partial r} \left( r^2 V_r \right) + \frac{1}{3r} \frac{\partial}{\partial \theta} \left( \sin \theta v_\theta \right) + k_p B^2 p \right] \\
z_f &= 2 k_p B^2 p.
\end{align*}
\]

As stated in Chapter 6, the axisymmetric transport equation (B.14) is solved over the interval \(0 \leq \theta \leq \pi\), while the numerical scheme requires the zero-gradient Neumann condition

\[
\frac{\partial f}{\partial \theta} = 0 \bigg|_{i,j=n_\theta}
\]

at both boundaries. It is therefore important to note that the coefficient \(z_\theta \to \infty\) as \(\theta \to 0\). This can be seen by expanding the second term in \(z_\theta:\)

\[
\frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \kappa_{\theta \theta} \right) = \frac{\cos \theta}{r^2 \sin \theta} \kappa_{\theta \theta} + \frac{1}{r^2} \frac{\partial \kappa_{\theta \theta}}{\partial \theta}.
\] (C.60)

This problem occurs only at the boundary, but can be removed by applying L’Hospital’s rule to the offending term

\[
\frac{\cos \theta}{r^2 \sin \theta} \kappa_{\theta \theta} \frac{\partial f}{\partial \theta} = \frac{\kappa_{\theta \theta} \frac{\partial f}{\partial \theta}}{r^2 \tan \theta}.
\] (C.61)

This is possible by virtue of the choice of \(\theta\) boundary condition. Applying the rule one finds that

\[
\lim_{\theta \to 0} \left[ \frac{\partial f}{\partial \theta} \left( \tan \theta \right)^{-1} \right] = \lim_{\theta \to 0} \left[ \frac{\partial^2 f}{\partial \theta^2} \cos^2 \theta \right] = \lim_{\theta \to 0} \frac{\partial^2 f}{\partial \theta^2}.
\] (C.62)
Therefore, at $\theta = 0$ the terms
\[
\frac{\kappa_{\theta \theta}}{r^2} \frac{\partial^2 f}{\partial \theta^2} + \left[ \frac{1}{r^2} \frac{\partial}{\partial r} (r \kappa_r) + \frac{\cos \theta}{r^2 \sin \theta} \kappa_{\theta \theta} + \frac{1}{r^2} \frac{\partial \kappa_{\theta \theta}}{\partial \theta} - \frac{v_\theta}{r} \right] \frac{\partial f}{\partial \theta}
\]
in the axisymmetric transport equation (B.14) are modified to become
\[
\frac{2\kappa_{\theta \theta}}{r^2} \frac{\partial^2 f}{\partial \theta^2} + \left[ \frac{1}{r^2} \frac{\partial}{\partial r} (r \kappa_r) + \frac{1}{r^2} \frac{\partial \kappa_{\theta \theta}}{\partial \theta} - \frac{v_\theta}{r} \right] \frac{\partial f}{\partial \theta}.
\]
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