Chapter 4

Numerical Methods

In Chapter 3 we have derived the linear system of PDEs (3.23) with respect to time $t$ and the radius $r$,

$$
\dot{y}'(t, r) - A(r)\dot{y}(t, r) = \xi(r) \left[ D(r)\dot{y}'(t, r) + E(r)y(t, r) \right],
$$

(4.1)

for the solution vector $y(t, r)$ describing the response of the spherically symmetric, viscoelastic, Maxwell Earth model. (The degree and order subscripts, $n$ and $m$, respectively, of $y_{nm}$, $A_n$, $D_n$ and $E_n$ are suppressed throughout this chapter.) Now we are concerned with numerical methods applicable to this system. We begin with a rather terminological remark on differential-algebraic equations which, in fact, precede (4.1). Among several possible techniques of solution to (4.1), we prefer and elaborate the semi-discretizing method of lines (MOL). We discuss two essences of MOL: semi-discretization of the system in the spatial dimension and a choice of methods for time integration of intermediate ODEs, often possessing a high degree of numerical stiffness. We adopt two stiff integrators based on Press et al. (1996)\(^1\). We also discuss another semi-discretizing method, the method of Rothe, employed in publications collected in Part II. Finally, numerical examples demonstrate the efficiency of the presented approach.

4.1 Differential-Algebraic Equations

Differential-algebraic equations (DAEs), features of DAEs and numerical techniques applicable to DAEs have been a subject of an intensive research over the recent years (see, e.g., Ascher & Petzold 1998 for thorough introduction and a bibliography). Since one of below mentioned techniques for dealing with DAEs has already been applied in Chapter 3, we bring a brief introduction into the terminology of DAEs. Our intent is to emphasize that the system of PDEs (4.1) is essentially based on a system of DAEs, and that techniques available within the DAE methodology should be examined in future works on the IV approach.

\(^1\)Our reference to Press et al. (1996) stands for either of Press et al. (1996a) and Press et al. (1996b). The former should be consulted for more details on theoretical background, more references and routines coded in Fortran 77, the latter for the same routines translated into Fortran 90.
where $F$ is a vector function with, possibly, a singular Jacobian matrix $\partial F/\partial \dot{y}$. (The dot means differentiation with respect to $t$. Within this chapter, the italicized $y$ is casted as an arbitrary vector in rather general statements; the solution vector $y$ to (4.1) is, however, the intended target.) The minimal number of differentiations of (4.2) which would be required to solve for $\dot{y}(t)$ uniquely in terms of $y(t)$ and $t$ is referred to as the index along the solution $y(t)$. In other words, the index of a system of DAEs is equal to a number of differentiations needed to obtain an explicit system of ODEs for $y(t)$; ODEs are index-0 DAEs. It should be noted that the classification of DAEs is still in evolution; e.g., the above defined index gives a partial insight as it can depend not only on the form of DAEs but also on local features of the solution $y(t)$.

Most DAEs encountered in practice can be written in the form

$$f(t, u, \dot{u}, v, \dot{v}) = 0,$$ (4.3)
$$g(t, u, v) = 0.$$ (4.4)

This system can also be referred to as the ODEs (4.3) with the algebraic constraints (4.4). The general treatment of DAEs usually begins by some reformulation. For the particular case of (4.3)–(4.4), at least two techniques are conceivable: substitution of, e.g., $v(t)$ from (4.4) into (4.3), which would yield ODEs for $u(t)$, and analytical differentiation of (4.4). The former technique can be applied when $v(t)$ is explicitly expressible from (4.4), the latter is eligible for low-index DAEs.

The number of differentiations of (4.4) equal to the index leads to the elimination of the algebraic part in the sense that the system of DAEs takes the form of a system of ODEs. The technique of analytical differentiation is referred to as index reduction.

From comparison of (4.3)–(4.4) with our system of the field PDEs (3.3)–(3.4) we see that the momentum equation forms a differential part of DAEs similar to (4.3), while the Poisson equation gives an algebraic part in the form of (4.4). (The spatial dependence is irrelevant in this context.) Thus, we can obtain the system of DAEs,

$$\dot{y}'_{1..4,7..8}(t,r) - A_{1..4,7..8 \times 1..8}(r)\dot{y}_{1..8}(t,r) - \\
- \xi(r) [D_{1..4,7..8 \times 1..8}(r)\dot{y}'_{1..8}(t,r) + E_{1..4,7..8 \times 1..8}(r)y_{1..8}(t,r)] = 0,$$ (4.5)
$$\dot{y}'_{5,6}(t,r) - A_{5,6 \times 1..8}(r)y_{1..8}(t,r) = 0,$$ (4.6)

where the subscripts $nm$ have been suppressed and the remaining subscripts denote the ranges of rows and columns. Differentiation of (4.6) with respect to $t$ gives (3.13) and (3.21) and leads consequently, with (4.5), to the PDEs (4.1).

We conclude that the field PDEs (3.3)–(3.4) give rise to the time-dependent linear index-1 system of DAEs (4.5)–(4.6) which in turn leads to the system of PDEs (4.1) by application of index reduction.

4.2 Method of Lines. Step 1: Discretization in Space

We describe the method of discretization of the PDEs (4.1). It is known that the solution vector $y(t,r)$ can be characterized by the exponential-like development in time and by the spatial distribution which can be expressed in terms of the spherical Bessel functions. In other words, the
behaviour of $y(t, r)$ is considerably different in the directions of each independent variable. For this kind of PDEs, methods based on semi-discretization are of a great benefit. Here we discuss the semi-discretizing method referred to as the method of lines. Applying the spatial discretization to (4.1), the intermediate system of ODEs (4.14) is derived. In this context, we point out to a procedure for the evaluation of weights of finite-difference (FD) formulas on arbitrarily spaced grids (Fornberg 1996). We briefly discuss (4.14) from the viewpoint of the eigenvalue analysis.

More or less detailed mentions of the MOL idea can be found in several textbooks (e.g., Dahlquist & Björck 1974; Ascher & Petzold 1998). Monographs concentrated on MOL appeared as well (e.g., Schiesser 1991).

4.2.1 Preliminary Notes on the Semi-discretizing Methods

Semi-discretizing methods for solution to the time- and spatially-dependent PDEs are based on decomposition of the process of discretization into two steps: discretization in space and discretization in time. Either of these steps leads first to intermediate ODEs, and second to algebraic equations. The actual sequence of the steps determines whether the intermediate ODEs form an initial-value (IV) problem or a boundary-value (BV) problem. The intent of the two-step discretization is to allow for utilization of specialized techniques designed for solution to the intermediate ODEs. These techniques accomplish the second, often trickier, or at least too routine, step of the process of solution.

Let us consider a system of $K$ PDEs for the $K$-element vector $y(t, r)$,

$$ F(t, r, y(t, r), y'(t, r), y''(t, r)) = 0, $$

(4.7)

with initial and boundary conditions $y(0, r) = y_0(r)$ and, e.g., $y(t, a) = y_a(t)$, $y(t, b) = y_b(t)$, respectively. The spatial discretization on the grid $r_0 = b < r_1 < \ldots < r_J = a$ and the substitution of FD formulas for the spatial derivatives converts (4.7) into the IV problem for ODEs,

$$ F^\text{IV}(t, y^\text{IV}(t), y'^\text{IV}(t)) = 0, $$

(4.8)

which is, in fact, a set of scalar IV problems to be integrated along the lines of constant grid points: we have arrived at the reason why MOL is called MOL (sometimes also the numerical method of lines, NUMOL). The $K \times (J + 1)$-element solution vector $y^\text{IV}(t)$ is composed of $y(t, r_0)$, $\ldots$, $y(t, r_J)$; the initial condition for $y^\text{IV}(0)$ is constructed from $y_0(r_0)$, $\ldots$, $y_0(r_J)$ in the same manner. The actual number of the ODEs (4.8) depends on the character of the boundary conditions. For the Dirichlet boundary conditions, i.e., those imposed on $y(t, a)$ and $y(t, b)$, the number of scalar unknowns is in fact $K \times (J - 1)$, and the same number of equations is necessary: ODEs (4.7) in the $J - 1$ interior grid points are to be employed. For the Neumann boundary conditions, i.e., those imposed on $y'(t, a)$ and $y'(t, b)$, the number of scalar unknowns remains $K \times (J + 1)$ and the discretized boundary conditions must be added to the $K \times (J - 1)$ equations in the interior points to reach the necessary number of equations, $K \times (J + 1)$. In the second step, numerical routines appropriate for solution to the IV problems for ODEs (the IV integrators) are applied to (4.8) what results in the above mentioned algebraic equations. It is the advance in the field of IV integrators what makes this approach particularly attractive. Essential prerequisites for efficiency of the integration, namely the adoption of stable integrators and adaptive stepsize control guided by required accuracy, are ensured on a user’s behalf by more or less standardized ODE packages.
### Table 4.1. Weights for centered FD formulas on an equally spaced grid (Fornberg 1996)

<table>
<thead>
<tr>
<th>order</th>
<th>$w_{j-4}$</th>
<th>$w_{j-3}$</th>
<th>$w_{j-2}$</th>
<th>$w_{j-1}$</th>
<th>$w_j$</th>
<th>$w_{j+1}$</th>
<th>$w_{j+2}$</th>
<th>$w_{j+3}$</th>
<th>$w_{j+4}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$\frac{1}{2}$</td>
<td>$0$</td>
<td>$\frac{1}{2}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>$-\frac{1}{12}$</td>
<td>$\frac{1}{6}$</td>
<td>$\frac{1}{2}$</td>
<td>$\frac{1}{6}$</td>
<td>$\frac{1}{12}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>$-\frac{1}{60}$</td>
<td>$\frac{3}{20}$</td>
<td>$\frac{1}{4}$</td>
<td>$\frac{3}{20}$</td>
<td>$\frac{1}{60}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>$\frac{1}{280}$</td>
<td>$-\frac{4}{105}$</td>
<td>$\frac{1}{5}$</td>
<td>$-\frac{4}{105}$</td>
<td>$\frac{1}{280}$</td>
<td></td>
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<td></td>
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</tr>
</tbody>
</table>

2nd derivative, $f''_j \approx \sum_{k=-4}^{4} w_{j+k} f_{j+k}/h^2$

<table>
<thead>
<tr>
<th>order</th>
<th>$w_{j-4}$</th>
<th>$w_{j-3}$</th>
<th>$w_{j-2}$</th>
<th>$w_{j-1}$</th>
<th>$w_j$</th>
<th>$w_{j+1}$</th>
<th>$w_{j+2}$</th>
<th>$w_{j+3}$</th>
<th>$w_{j+4}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$1$</td>
<td>$-2$</td>
<td>$1$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>$-\frac{1}{12}$</td>
<td>$\frac{4}{7}$</td>
<td>$-\frac{1}{2}$</td>
<td>$\frac{4}{7}$</td>
<td>$\frac{1}{12}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>$\frac{1}{60}$</td>
<td>$-\frac{3}{20}$</td>
<td>$\frac{3}{20}$</td>
<td>$\frac{1}{60}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>$-\frac{1}{560}$</td>
<td>$\frac{8}{315}$</td>
<td>$-\frac{1}{20}$</td>
<td>$\frac{8}{315}$</td>
<td>$-\frac{1}{560}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

On the other hand, the idea of another semi-discretizing method, called the method of Rothe, is to discretize the PDEs (4.7) in time, $t_0 = 0 < t_1 < \ldots < t_i < \ldots$ It results in a series of BV problems for ODEs parametrized by the time index $i$,

$$F^{BV}(i, r, y^{BV}(i, r), y^{BV'}(i, r)) = 0,$$

for the $K$-element solution vector $y^{BV}(i, r)$, with the boundary conditions $y^{BV}(i, a) = y_a(i)$ and $y^{BV}(i, b) = y_b(i)$. Since $F^{BV}$ depends, at least implicitly, on the integration history, eq. (4.9) is to be solved successively for $i = 0, 1, \ldots$ For the apparent “orthogonality” to MOL, the method of Rothe is occasionally referred to as the transverse method of lines.

We have already stated that MOL will be particularly suitable if the solution behaves considerably different along the directions of each dimension. Following Ascher & Petzold (1998), another feature of the solution should also signal the advisable application of MOL: if no sharp fronts move rapidly in both space and time, i.e., if these fronts, if they exist, can be reasonably well decoupled in the both dimensions. Hence, MOL is thought to be more suitable for the parabolic PDEs than for the hyperbolic ones, although successful MOL applications are developed for the both classes of PDEs (and—not only as a curiosity—MOL applications for solving to the elliptic PDEs have also been proposed, e.g., Schiesser 1991). We remind that PDEs (4.1) involve the first derivatives with respect to time explicitly and the second derivatives with respect to the radius implicitly, through the stress components of $y$. Thus, PDEs (4.1) can be characterized as the parabolic PDEs.

A final preliminary note: beside the semi-discretizing methods, universal FD techniques for discretization in the both dimensions in parallel can be applied to (4.1). However, the standard FD schemes lack the efficiency for the stiff problems. To our present knowledge, the IV integrators are the only methods which appear to be capable for solution to the stiff problems. Thus, we adhere to them in what follows.
4.2.2 Finite-Difference Formulas on Arbitrarily Spaced Grids

The derivatives can be approximated by FD formulas which weights are either tabulated a priori or are evaluated by means of a numerical routine. The former eventuality is reasonably applicable to equally spaced grids, while the latter is general and can be applied to arbitrarily spaced grids. In the latter case, the weights are dependent on the grid-point locations.

In Table 4.1 we gather the weights of the centered FD formulas of various orders of accuracy for the first and the second derivatives of \( f(x) \) at the point \( x_j \), \( f_j' \equiv f'(x_j) \) and similarly for \( f_j'' \), in terms of values \( f_{j+k} \equiv f(x_{j+k}) \), \( k = 0, \pm 1, \ldots \), in adjacent, equally spaced grid points \( x_{j+1}, x_{j-1}, x_{j+2}, x_{j-2} \) etc. In Table 4.2 the one-sided approximations in terms of values of \( f(x) \) at \( x_j, x_{j+1}, x_{j+2} \) etc. are collected. To give an example, the second-order FD formulas for the first derivative of \( f(x) \) take the form as follows,

\[
f_j' \approx \frac{-f_{j-1} + f_{j+1}}{2h} \approx -\frac{3f_j + 4f_{j+1} - f_{j+2}}{2h} \approx \frac{f_{j-2} - 4f_{j-1} - 3f_j}{2h},
\]

with \( h = x_{j+1} - x_j = x_j - x_{j-1} \).

An efficient algorithm for the evaluation of the weights of the FD formulas for arbitrary derivatives of \( f(x) \) was discovered and first published by Fornberg in 1988. The weights are obtained by
differentiation of the Lagrange interpolating polynomial fitting a set of arbitrary nonrepeated points and by utilization of some recursion relations. The algorithm has been described in both a symbolic language and Fortran 77 in Fornberg (1996) and we rewrite it in Fortran 90 in Appendix C.1.

4.2.3 Discretized System of Ordinary Differential Equations

In order to present a compact numerical formulation of the IV/MOL approach, we discretize the PDEs (4.1) in the spatial dimension using the second-order FD formulas. However, FD formulas of higher orders could be employed in a similar manner.

On the arbitrarily spaced grid, \( x_0 = b < x_1 < \ldots < x_J = a \), we can write the second-order FD formulas for the first derivative of \( f(x) \) in the general form,

\[
\begin{align*}
    f'_0 &\approx \beta_0 f_0 + \gamma_0 f_1 + \alpha_0 f_2, \\
    f'_j &\approx \alpha_j f_{j-1} + \beta_j f_j + \gamma_j f_{j+1}, \quad j = 1, 2, \ldots, J - 1, \\
    f'_J &\approx \gamma_J f_J + \alpha_J f_{J-1} + \beta_J f_J,
\end{align*}
\]

(4.11–4.13)

where \( \alpha_j, \beta_j \) and \( \gamma_j, j = 0, \ldots, J \), are the weights discussed above. For \( x_{j+1} - x_j = x_j - x_{j-1} \), eqs (4.11–4.13) reduce to (4.10).

Let us consider (4.1) in an interior point \( x_j \). With FD formulas by (4.11–4.13), the term \( \dot{y}_j \) is approximated by \( \alpha_j \dot{y}_{j-1} + \beta_j \dot{y}_j + \gamma_j \dot{y}_{j+1} \), similarly \( D \dot{y} \approx D_j (\alpha_j y_{j-1} + \beta_j y_j + \gamma_j y_{j+1}) \), etc. It becomes apparent that (4.1) discretized with respect to \( r \) can be expressed in the form of the ODEs for the solution vector \( y(t) \),

\[
P \dot{y}(t) = Q y(t) + q.
\]

(4.14)

Vector \( y(t) \) consists of \( 8 \times (J + 1) \) elements,

\[
y(t) = \begin{bmatrix} y_0 & y_1 & \ldots & y_J \end{bmatrix},
\]

(4.15)

where each block represents one 8-element vector \( y_j \equiv y(t, r_j), \ j = 0, \ldots, J \). Matrix \( P \) is band-diagonal with constant coefficients and made from \( 8 \times 8 \) blocks. It can be schematically sketched in the form of \( J + 1 \) block-rows and the same number of block-columns, as follows:

\[
P = \begin{pmatrix}
\beta_0 I - A_0 & \gamma_0 I & \alpha_0 I & & & & & & & & & & & & & & \\
\alpha_1 I & \beta_1 I - A_1 & \gamma_1 I & & & & & & & & & & & & & & \\
\alpha_2 I & \beta_2 I - A_2 & \gamma_2 I & & & & & & & & & & & & & & \\
& & & & & & & & & & & & & & & & \\
& & & & & & & & & & & & & & & &
\end{pmatrix},
\]

(4.16)

where \( I \) is the diagonal matrix and \( A_j \equiv A(r_j), \ j = 0, \ldots, J \). Focussing the attention to the specific, i.e., diagonal shape of the two thinly framed blocks, \( \alpha_0 I \) and \( \gamma_J I \), these blocks can be eliminated.
by subtraction of the appropriately multiplied adjacent block-rows, i.e., those with $\gamma_I I$ and $\alpha_{J-1} I$, respectively. Matrix $Q$ is band-diagonal, too, and can be sketched in the similar manner,

$$Q = \begin{pmatrix}
\beta_0 D_0 + E_0 & \gamma_0 D_0 & \alpha_0 D_0 \\
\alpha_1 D_1 & \beta_1 D_1 + E_1 & \gamma_1 D_1 \\
\alpha_2 D_2 & \beta_2 D_2 + E_2 & \gamma_2 D_2 \\
& \ddots & \ddots & \ddots \\
\alpha_{J-1} D_{J-1} & \beta_{J-1} D_{J-1} + E_{J-1} & \gamma_{J-1} D_{J-1} \\
0 & \gamma_J D_J & \alpha_J D_J & \beta_J D_J + E_J
\end{pmatrix}, \quad (4.17)$$

where (sic) $D_j \equiv \xi(r_j)D(r_j)$ and $E_j \equiv \xi(r_j)E(r_j)$, $j = 0, \ldots, J$. The elimination of the off-diagonal blocks is only feasible if all corresponding elements of the adjacent blocks are mutually proportional. This has been the case of the diagonally-shaped blocks, but it might not be the case of the blocks $\alpha_0 D_0$ and $\gamma_J D_J$ versus $\gamma_1 D_1$ and $\alpha_{J-1} D_{J-1}$. However, setting $D_0 = D_1$ and $D_J = D_{J-1}$ seems to be a satisfactory approximation; a possibility to discretize more densely near the boundaries is congenial in this context.

The r.h.s. vector $q$ has the same block structure as is shown in (4.15). A description of the explicit shape of $q$ must be preceded by some remarks on the treatment of the boundary conditions. At $r = r_J = a$, $a$ is the radius of the Earth, we employ the boundary conditions by (3.26), i.e., those by Farrell (1972) with the Heaviside dependence in time. In the $J$th and $(J-1)$th block-rows, we (i) eliminate the 3rd, 4th, 6th and 8th elements of $y_J$ from the solution vector $y(t)$, shortening so its length, (ii) substitute the eliminated elements of $y_J$ into the $Qy(t)$ term, (iii) eliminate the 3rd, 4th, 6th and 8th rows of the $J$th block-row in (4.14); preserved equations correspond, in fact, to the discretized Neumann boundary conditions (cf. p. 31). Steps (i) and (ii) result in some constant terms which emerge in the equations of the $J$th and $(J-1)$th block-rows and must be moved to the r.h.s. Thus, we receive 12 elements of $q$, 8 in the block $q_{J-1}$ and 4 in the truncated block $q_J$. The boundary conditions at $r = r_0 = b$, i.e., at the core-mantle boundary, should be deduced from the general requirements for the liquid boundaries, see p. 11 and 19. A special treatment would require the case of $b = 0$ which is examined in Section 4.5. For now we skip further discussion of the boundary conditions at $r = b$, leaving the only note that they may contribute to the blocks $q_0$ and $q_1$. The other blocks $q_j$, $j = 2, \ldots, J-2$, are zero identically.

In (4.14) we have arrived at the linear, band-diagonal ODEs with constant coefficients. Note that the spheroidal and toroidal parts of (4.14) remain decoupled and that it is necessary only to solve the spheroidal part if the boundary conditions (3.26) are considered. The form of (4.14) is appropriate for the application of standard IV integrators. This is discussed in detail in Section 4.3.

### 4.2.4 Eigenvalue Analysis

We make an ancillary note on the role of the eigenvalue analysis for studying relaxation spectra of the Earth models. For the linear homogeneous system of ODEs with constant coefficients,

$$\dot{y}(t) = By(t), \quad (4.18)$$

...
with $B$ the constant matrix, a solution, referred to as the fundamental system, can be written as a linear combination of the constituents

$$e^{\lambda_p t} \quad \text{or} \quad R_q e^{\lambda_q t},$$

where $\lambda_p$ is any nondegenerated eigenvalue of $B$, $\lambda_q$ any $Q$-degenerated eigenvalue of $B$ and $R_q$ a polynomial of the maximal degree $Q - 1$. For the nonhomogeneous system of ODEs,

$$\dot{y}(t) = By(t) + b,$$  \hspace{1cm} (4.20)

a solution is the sum of the fundamental system and a particular solution; for constant $b$ the particular solution is constant, too. If there is any (complex) eigenvalue $\lambda_r$ of $B$ with a positive real part, the fundamental system of (4.20) will contain a term with $e^{\Re \lambda_r t}$, and the solution will be exponentially growing with increasing $t$.

The ODEs (4.14) form the linear nonhomogeneous system with constant coefficients and, for the surface boundary conditions (3.26), with the constant r.h.s. vector $q$. In comparison with (4.20) we see that

$$y(t) = y(t), \quad B = P^{-1}Q, \quad b = P^{-1}q.$$  \hspace{1cm} (4.21)

It follows from the statements given above that it is possible to study the properties of the solution to (4.14) by means of the eigenvalue analysis applied to $B = P^{-1}Q$. This technique is certainly related to the traditional normal-mode technique by Peltier (1974). However, if the relaxation times—or stability of the initial model—are only concerned, it might be convenient to construct matrices $P$ and $Q$ and to subject $B = P^{-1}Q$ to some routines from standard eigenvalue packages.

Unfortunately, numerical routines for the evaluation of eigenvalues are only efficient for symmetric or Hermitian matrices. For nonsymmetric matrices, the numerical demands, in terms of the processing time, are growing with the third power of the size of matrices. The reasonable bound on $J$, the total number of layers of the spatial grid discussed above, could not exceed few hundreds.

The appropriate routines for solution to eigenvalues of real nonsymmetric matrices are \texttt{balanc}, \texttt{eigenv}, and \texttt{hqr} by Press et al. (1996). It might be profitable to browse other, specialized libraries (e.g., LAPACK/EISPACK\textsuperscript{2}).

### 4.3 Method of Lines. Step 2: Integration in Time

In the previous section the intermediate system of ODEs (4.14) with respect to time has been derived by application of the spatial discretization to PDEs (4.1). It is a general feature of MOL that the intermediate ODEs possess a high degree of numerical stiffness. We begin this section by the illumination of the concept of stiffness. Then, two methods appropriate for integrating stiff ODEs (referred to as the stiff integrators) are introduced and adapted for the band-diagonal structure of the ODEs (4.14). Numerical routines for solution to the underlying linear algebraic equations with the band-diagonal structure are proposed.

\textsuperscript{2}In http://www.netlib.org.
4.3.1 Concept of Stiffness

Stiffness occurs in a problem where there are two or more very different scales of the independent variable on which the dependent variables are changing. We encounter two sources of numerical stiffness within the IV/MOL approach: (i) that of the physical origin which appears when physical parameters (viscosity, in particular) of the Earth model under consideration span over several orders of magnitude, and (ii) that somehow intrinsic to MOL applications, emergent from the spatial discretization. While the time scale of a problem is determined by the smallest eigenvalue, the largest eigenvalue multiplied by the stepsize in time must lie in the region of the absolute stability of the integration scheme. These regions of explicit integration schemes are generally substantially smaller than those of implicit schemes. It is a problem of stability rather than accuracy what handicaps the explicit schemes in stiff problems.

The origin of stiffness can be demonstrated by the classic example (e.g., Press et al. 1996a). Let us consider the single ODE

\[ \dot{y} = -cy \]  

with constant \( c > 0 \) and the solution \( y(t) = Ae^{-ct} \) with \( A \) given by an initial value. The explicit Euler scheme leads to

\[ y_{n+1} = y_n + hy'_n = (1 - ch)y_n, \]  

with \( h = t_{n+1} - t_n \), while the implicit Euler scheme gives

\[ y_{n+1} = y_n + hy'_{n+1} = \frac{y_n}{1 + ch}. \]  

While the former scheme becomes unstable for \( h > 2/c \), since \( |y_{n+1}| > |y_n| \) for any \( n \) and \( y_n \) and \( \lim_{n \to \infty} y_n \to \infty \), the latter formula gives the correct value of \( \lim_{n \to \infty} y_n \) even for \( h \to \infty \). Analogically for the linear system of ODEs with constant coefficients,

\[ \dot{y} = -Cy, \]  

with \( C \) the positive definite matrix (i.e., with positive eigenvalues), the condition of stability imposed on the largest allowed step of explicit Euler differencing is \( h < 2/\lambda_{\text{max}} \), where \( \lambda_{\text{max}} \) is the largest eigenvalue of \( C \). The long-time character of the relaxation of \( y \), proportional to \( \exp(-\lambda_{\text{min}}t) \), can only be traced by explicit schemes with stepsizes given above. The shortcomings of this constraint for the stiff problems, with the ratio of \( \lambda_{\text{max}}/\lambda_{\text{min}} \) being large, are apparent. On the other hand, implicit Euler differencing applied to (4.25) retains stability for all stepsizes \( h \).

Turning to the implicit schemes, a question of accuracy receives the priority. For instance, the implicit Euler scheme, with the region of absolute stability spanning over the complex plane with the exception of the unit circle around the point (1,0), is only first-order accurate. In the following we introduce efficient higher-order methods for integrating IV problems for stiff ODEs in the general form of

\[ \dot{y} = f(t, y), \quad y(t_0) = y_0. \]  

Several classes of higher-order methods have been proposed (e.g., Ascher & Petzold 1998). First we describe generalizations of the Runge-Kutta method, namely the Rosenbrock methods (also called

\[ \begin{align*}
\end{align*} \]
Chapter 4

the Kaps-Rentrop methods). Second, we turn to generalizations of the Bulirsch-Stoer methods referred to as the semi-implicit extrapolation methods. The other class (from the historical point of view, the first one) covers predictor-corrector methods usually based on the Gear multistep backward differentiation formulas. Press et al. (1996) confine themselves to the single-step methods of the first two classes, and so do we. A particular reason for this choice is the larger memory consumption of the multistep methods what can become prohibitive in 2-D and 3-D modelling.

4.3.2 Rosenbrock Method

Let us remind the general scheme of the Runge-Kutta methods for integrating ODEs (4.26), e.g., Ascher & Petzold (1998),

\[
y(t_0 + h) = y_0 + \sum_{i=1}^{s} c_i k_i, \quad k_i = hf \left( y_0 + \sum_{j=1}^{i-1} \alpha_{ij} k_j \right), \quad i = 1, \ldots, s, \tag{4.27}
\]

with \( h \) the stepsize and \( c_i \) and \( \alpha_{ij} \) constants of a particular member of the Runge-Kutta family. In the Rosenbrock methods, vectors \( k_i \) are the solutions to \( s \) linear algebraic equations

\[
(I - \gamma h f') \cdot k_i = hf \left( y_0 + \sum_{j=1}^{i-1} \alpha_{ij} k_j \right) + h f' \cdot \sum_{j=1}^{i-1} \gamma_{ij} k_j, \quad i = 1, \ldots, s, \tag{4.28}
\]

where \( f' \equiv \partial f / \partial y \) denotes the Jacobian matrix and the coefficients \( c_i, \gamma, \alpha_{ij} \) and \( \gamma_{ij} \) are constants of a particular member of the Rosenbrock family. Note that for \( \gamma = \gamma_{ij} = 0 \), eqs (4.28) reduce to the Runge-Kutta scheme (4.27). The algorithm for the automatic stepsize adjustment in the Rosenbrock methods became available by the Kaps-Rentrop (or, later, Shampine) implementation of the embedded, Runge-Kutta-Fehlberg schemes (and is also implemented by Press et al. 1996).

Let us recall that the ODEs (4.14) can be casted into (4.26) with

\[
\begin{align*}
f &= P^{-1}(Qy + q), \tag{4.29} \\
f' &= P^{-1}Q. \tag{4.30}
\end{align*}
\]

For (4.29)–(4.30), it is advisable to rewrite the Rosenbrock scheme (4.28) into the form

\[
(P - \gamma h Q) \cdot k_i = h \left[ Q \left( y_0 + \sum_{j=1}^{i-1} \alpha_{ij} k_j \right) + q \right] + hQ \cdot \sum_{j=1}^{i-1} \gamma_{ij} k_j, \quad i = 1, \ldots, s, \tag{4.31}
\]

where the band-diagonal matrices appear on the both sides. Press et al. (1996) have implemented the Rosenbrock stiff integrator for (4.28) by the routine stiff. We need a modified implementation for the special, band-diagonal form of both sides of (4.31). This can be found in Appendix C.2.

4.3.3 Semi-implicit Extrapolation Method

The original Bulirch-Stoer extrapolation method based on the modified midpoint rule and the idea of Richardson extrapolation has been accommodated to the stiff problems by inventing a new, semi-implicit midpoint rule. Press et al. (1996a) give details, references and the implementation. We adjust here this method to the ODEs (4.14).
First, we give in two sentences the outline of the Bulirsch-Stoer method. The method extrapolates a value of \( y(t + H) \) from estimations of \( y(t + H) \), obtained by the evaluation of a series of \( n \)-step progressions of \( y_k \equiv y(t + kh) \), \( h = H/n \), \( k = 1, \ldots, n \). In other words, one computes an estimate of \( y(t + H) \) using the midpoint rule with \( n_1 \) equidistant steps \( h_1 = H/n_1 \), then another estimate of \( y(t + H) \) with \( n_2 \) equidistant steps \( h_2 = H/n_2 \), \( h_2 < h_1 \), etc., as far as the method asks for, and then an estimate corresponding to \( h \to 0 \) is extrapolated. Second, we show the implementation of the semi-implicit midpoint rule by Press et al. (1996). With \( \Delta_k = y_{k+1} - y_k \) and \( h = H/m \), the implementation for the general ODEs (4.26) takes the following form,

\[
\begin{align*}
\Delta_0 &= (I - hf')^{-1} \cdot hf(y_0), \\
\Delta_k &= \Delta_{k-1} + 2 (I - hf')^{-1} \cdot [hf(y_k) - \Delta_{k-1}], \\
\Delta_m &= (I - hf')^{-1} \cdot [hf(y_m) - \Delta_{m-1}], \\
\end{align*}
\]

\( y_1 = y_0 + \Delta_0, \quad y_{k+1} = y_k + \Delta_k, \quad y_m = y_m + \Delta_m. \)

Third, we rewrite (4.32) for the ODEs (4.14), i.e., we substitute for \( f \) and \( f' \) from (4.29)–(4.30):

\[
\begin{align*}
(P - hQ) \Delta_0 &= h(Qy_0 + q), \\
(P - hQ) \Delta_k &= (P - hQ) \Delta_{k-1} + 2 [h(Qy_k + q) - P \Delta_{k-1}], \\
(P - hQ) \Delta_m &= [h(Qy_m + q) - P \Delta_{m-1}],
\end{align*}
\]

\( y_1 = y_0 + \Delta_0, \quad y_{k+1} = y_k + \Delta_k, \quad y_m = y_m + \Delta_m. \)

Note that we refer here by \( y_k, k = 0, \ldots, m \), to the values of \( y(t) \) at the internal stages of the Bulirsch-Stoer method, not to the block components of \( y(t) \) in (4.15). The implementation of the semi-implicit extrapolation stiff integrator is available in Press et al. (1996) by the routine \texttt{stifbs}. To adapt \texttt{stifbs} to (4.33), a part of the routine for solution to (4.32) has to be rewritten; a part controlling the automatic stepsize adjustment can be preserved without any change.

### 4.3.4 Linear Algebraic Equations

We have arrived at the systems of linear algebraic equations (4.31) and (4.33) to which the Rosenbrock and the semi-implicit extrapolation stiff integrators, respectively, reduce the ODEs (4.14). We see that at each time step, one algebraic system with the matrix \( P - hQ \) must be solved repeatedly for several different r.h.s. (Multiplier \( \gamma \) from (4.31) is irrelevant here.) Matrices \( P \) and \( Q \) are constant and given by (4.16) and (4.17), respectively, vector \( q \) depends on imposed boundary conditions. It is a crucial property of this algebraic system that \( P - hQ \) is a band-diagonal matrix and that band-diagonal solvers may be applied. Numerical characteristics (both processing time and required memory) thus become linear functions of the number of spatial grid points.

Each block-row of \( P - hQ \) consists of three non-zero \( 8 \times 8 \) blocks, so the maximal width of the diagonal band is bounded by \( 15 + 1 + 15 = 31 \) elements at the most. For the spheroidal subsystem, which consists of \( 6 \times 6 \) blocks, the maximal width is bounded by \( 11 + 1 + 11 = 23 \) elements. Moreover, the off-diagonal blocks, essentially matrices \( I \) and \( D_j \), are either diagonal or sparse, cf. (3.24), so the actual width for the spheroidal subsystem amounts to \( 9 + 1 + 6 = 16 \) elements. In this context we remind the necessity of the reduction of the “off-off-diagonal” blocks \( \alpha_0 I, \gamma_j I, \alpha_0 D_0 \) and \( \gamma_j D_j \), see p. 34, otherwise the maximal width would be spuriously increased. Solvers to the algebraic band-diagonal equations are available anywhere (e.g., LAPACK\(^4\)). We adhere to

\[^4\text{In } http://www.netlib.org.\]
the pivoting solver by Press et al. (1996), \texttt{bandec} & \texttt{banbk}s, accompanied with the routine \texttt{banmul} for multiplication of a band-diagonal matrix by a vector to carry out the evaluation of the r.h.s. of (4.31) or (4.33).

The block structure of the diagonal band of $P - hQ$ allures to employ solvers which would exploit this feature. Matrices of this structure are referred to as block-diagonal and emerge commonly when FD formulas are applied to differential equations; the resulting algebraic equations are called the finite-difference equations. An appropriate solver based on Gaussian elimination can be found in Press et al. (1996) in the context of solving BV problems of ODEs by relaxation methods. Their routine \texttt{solvde} is designed for a rather special kind of finite-difference equations, the key internal routines \texttt{pinvs} and \texttt{red}, however, are applicable and, on account of the detailed description of this solver in the referenced source, the generalization (not presented here) is conceivable.

The part of the Rosenbrock stiff integrator, which solves to the algebraic system (4.31) by the band-diagonal solver \texttt{bandec} & \texttt{banbk}s and is intended as the replacement of the corresponding part of the routine \texttt{stiff} by Press et al. (1996), is presented in Appendix C.2.

### 4.4 Method of Rothe

Our older formulation of the IV approach is not based on MOL. In Section 3.1.4 we have demonstrated the compatibility of certain relations of both the older and the IV/MOL formulations. We show now that the older formulation is equivalent to the application of the method of Rothe (MOR) to the PDEs (4.1). MOR is favoured in theoretical studies on stability, uniqueness etc. of various kinds of evolutionary PDEs (e.g., Rektorys 1982). The characteristic feature of MOR is that discretization of PDEs in time is performed at first. This kind of discretization in time can not devote too much attention to the nature of PDEs, and, typically, MOR is not a particularly effective method for numerical solution to differential systems with a higher degree of stiffness. However, results presented in Chapters 5–8 have been computed using the older formulation, and we present here how it can be derived via MOR.

We consider the PDEs (4.1) in the form of (3.22) and without indicating the $r$-dependence of the quantities,

$$
\dot{\mathbf{y}}(t) - \mathbf{A}\mathbf{y}(t) = \mathbf{\xi} = \begin{pmatrix}
\frac{a_{13}(y_3(t) - KX(t))}{a_{24}y_4(t)} \\
-\frac{y_4(t) + \sum_k a_{3k}y_k(t) - b_{31}y_1(t) - b_{32}y_2(t) - b_{33}KX(t)}{0} \\
-\frac{y_3(t) + \sum_k a_{4k}y_k(t) - b_{41}y_1(t) - b_{42}y_2(t) - (b_{43} + 1/r) KX(t)}{0} \\
0 \\
0 \\
\frac{a_{78}y_8(t)}{0} \\
-\frac{y_8(t) + \sum_k a_{8k}y_k(t) - b_{87}y_7(t)}{0}
\end{pmatrix}. \quad (4.34)
$$

In Chapters 5 and 6 we have employed the first-order (Euler) explicit FD formula for the first derivative of the function $f(t)$, $f' \equiv f(t')$, ...
\[
\dot{f}(t^i) \approx \frac{f^{i+1} - f^i}{\Delta t^i}, \quad \Delta t^i \equiv t^{i+1} - t^i, \quad (4.35)
\]
cf. (5.3) and (6.3). Applying (4.35) to the time derivatives in (4.34), we obtain at \(t = t^i\)
\[
(y^{i+1})' - Ay^{i+1} = (y^i)' - Ay^i - \xi \Delta t^i
\]
\[
\begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
(y^i)' - \sum_k a_{3k} y_k^i & (y^i)' - \sum_k a_{4k} y_k^i & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{pmatrix}
\]

With \(a_{13}, \ldots, b_{87}\) substituted from (2.34)–(2.47), we arrive at the relation for \(q' = (y^{i+1})' - Ay^{i+1}\), cf. (6.22),
\[
q' = q^{i-1} + \xi \Delta t^i
\]
which conforms with (6.39).

Finally we discuss the integro-differential formulation presented in Chapter 7. We discretize (4.1) in time using the FD formula corresponding to (7.40), rewritten in the differential form as
\[
\omega \dot{f}^i + (1 - \omega) \dot{f}^{i+1} \approx \frac{f^{i+1} - f^i}{\Delta t^i}, \quad \Delta t^i \equiv t^{i+1} - t^i, \quad 0 \leq \omega \leq 1. \quad (4.37)
\]
Let us restrict ourselves to the special case of \(\omega = 0\), i.e., the purely implicit scheme. We obtain at the time level \(t = t^{i+1}\)
\[
(y^{i+1})' - Ay^{i+1} = (y^i)' - Ay^i + \xi \Delta t^i \left[D(y^{i+1})' + Ey^{i+1}\right], \quad (4.38)
\]
from what the relation for vector \(q^{i+1} = (y^{i+1})' - Ay^{i+1}\) follows immediately,
\[
q^{i+1} = q^i + \xi \Delta t^i \left[D(Ay^{i+1} + q^{i+1}) + Ey^{i+1}\right] = q^i + \xi \Delta t^i \left[(DA + E)y^{i+1} + Dq^{i+1}\right]. \quad (4.39)
\]
With the relations (3.62) for \(\bar{Q}_n\) and \(\tilde{Q}_n\), we have arrived at (7.43) with \(\omega = 0\), and, hence, at (7.45), the final expression of Chapter 7.
Table 4.3. Physical Parameters of the Homogeneous Earth Model and Other Constants

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>radius ( a )</td>
<td>6371 km</td>
</tr>
<tr>
<td>density ( \varrho_0 )</td>
<td>5517 \text{ kg m}^{-3}</td>
</tr>
<tr>
<td>Lamé elastic parameter ( \lambda )</td>
<td>(3.5288 \times 10^{11}) \text{ Pa}</td>
</tr>
<tr>
<td>shear modulus ( \mu )</td>
<td>(1.4519 \times 10^{11}) \text{ Pa}</td>
</tr>
<tr>
<td>bulk modulus ( K )</td>
<td>(4.4967 \times 10^{11}) \text{ Pa}</td>
</tr>
<tr>
<td>viscosity ( \eta )</td>
<td>(10^{21}) \text{ Pa s}</td>
</tr>
<tr>
<td>( \beta )</td>
<td>(\lambda + 2\mu)</td>
</tr>
<tr>
<td>( \gamma )</td>
<td>(3\mu K/\beta)</td>
</tr>
<tr>
<td>( \xi )</td>
<td>(\mu/\eta)</td>
</tr>
<tr>
<td>Newton gravitational constant ( G )</td>
<td>(6.6732 \times 10^{-11}) \text{ m}^3 \text{s}^{-2} \text{kg}^{-1}</td>
</tr>
<tr>
<td>year</td>
<td>(3600 \times 24 \times 365.25) \text{ s}</td>
</tr>
<tr>
<td>( \pi ) in \text{REAL(8)} data type of Fortran 90</td>
<td>3.141592653589793_8</td>
</tr>
</tbody>
</table>

4.5 Numerical Implementation

We illustrate the IV/MOL formulation by some output of the numerical modelling. Our current implementation targets on the homogeneous, spherically symmetric, Maxwell viscoelastic Earth models, both incompressible and compressible. We are not ready to release results for viscoelastic Maxwell models with realistic profiles of parameters or for models with the axially symmetric viscosity for the time being, the results below are, however, still worth to be presented since analytical solutions are known for the response of the homogeneous models. With what is given below, the means of validation of the new formulation is provided and the potential of the new code can be appraised.

The code solves to the spheroidal part of the ODEs (4.14) with constant matrices \( P \), \( Q \) and vector \( q \), all evaluated from \( A(r_j), D(r_j) \) and \( E(r_j) \) by (2.50), (3.24) and (3.25), respectively. Spatial grid points may be distributed arbitrarily, \( r_0 = b < r_1 < \ldots < r_J = a \), with \( a \) the radius of the model and \( b \) the radius of the elastic “core”, underlying the viscoelastic “mantle”. The boundary conditions at \( r = a \) have been imposed on \( y(t,a) = y_J(t) \) in accord with (3.26). A temporary shortage of the code resides in the adoption of the boundary conditions at \( r = b \). The outputs below have been obtained with the ad hoc choice of \( b = 0 \) and \( y(t,b) \equiv y_0(t) = 0 \), which partially complies with the initial elastic solution (3.27). It is apparent from Fig. 4.4 that this choice is essentially correct for \( y_0(t) \) at degrees \( n > 2 \) and for the non-stress components of \( y_0(t) \) at \( n = 2 \). The ODEs (4.14) have been solved by both the Rosenbrock and the semi-implicit extrapolation stiff integrators adapted for solution to (4.31) and (4.33), respectively. We have employed the Earth model defined by the constant values of initial density \( \varrho_0 \), elastic Lamé parameters \( \lambda \) and \( \mu \), and viscosity \( \eta \), according to Table 4.3. The gravitational acceleration can be deduced from (2.4), \( g_0(r) = \frac{4}{3}\pi G \varrho_0 r \). Let us also recall that, in the case of material incompressibility, \( \lambda \rightarrow \infty, K \rightarrow \infty, 1/\beta \rightarrow 0, \lambda/\beta \rightarrow 1 \) and \( \gamma \rightarrow 3\mu \).

In Fig. 4.1 we demonstrate the time evolution of the surface values of the Love numbers \( h_n, l_n \) and \( k_n, n = 2, 6, 15, 60 \) and 120, for the first \( 10^6 \) yr after the onset of the Heaviside (in time) point mass load at the surface. The surface Love numbers are related to the 1st, 2nd and 5th elements of \( y_J(t) \) by the definition (Farrell 1972)
Fig. 4.1. Time evolution of the surface Love numbers $h_n$, $l_n$ and $k_n$, $n = 2, 6, 15, 60$ and $120$, of the homogeneous incompressible model evaluated by the IV/MOL approach. One symbol represents one time step made by the Rosenbrock stiff integrator. The responses have been calculated with various density of the spatial discretization: symbols $\triangle$ denote values obtained with 11 equidistant spatial grid points (!), $+$ pertain to 101 grid points and $\times$ to 1001 grid points ($J = 10, 100$ and 1000, respectively). The equilibrium state is reached with less than 20 time steps; with 101 grid points, recent Pentium processors generate 20 time steps per second.
Fig. 4.2. Time evolution of the surface Love numbers $h_n$, $l_n$ and $k_n$, $n = 2, 6$ and 15, of the homogeneous incompressible model calculated by the semi-implicit extrapolation stiff integrator. One symbol represents one time step. The stepsizes are more than three times longer than in Fig. 4.1, the total evaluation time amounts to half.

\[
\begin{pmatrix}
y_{J,1} \\
y_{J,2} \\
y_{J,5}
\end{pmatrix} = \frac{\Phi_n}{N_n} \begin{pmatrix} h_n/g_0 \\ l_n/g_0 \\ -k_n
\end{pmatrix}, \quad \Phi_n = \frac{4\pi Ga}{2n+1}, \quad N_n = \sqrt{\frac{2n+1}{4\pi}}, \quad \Gamma_n = \frac{2n+1}{4\pi a^2}, \quad ... (4.40)
\]

with $\Phi_n$ the coefficients of the spherical harmonic expansion of the surface potential of the point mass load and $N_n$ the norm factors of the spherical harmonics, cf. (2.52). Let us remind that the 3rd, 4th and 6th elements of $y_J(t)$ are prescribed by the surface boundary conditions (3.26) and that we refrain from solution to the toroidal subsystem (7th and 8th elements). Symbols $\triangle$, $+$ and $\times$ in Fig. 4.1 and others represent the time instants, chosen automatically by the stiff integrators; each time instant is depicted. We have employed 11, 101 and 1001 equally spaced grid points in the spatial dimension (i.e., $J = 10$, 100 and 1000, respectively). The Rosenbrock stiff integrator has been launched for generating Fig. 4.1 and the semi-implicit extrapolation stiff integrator has been employed to compute responses in Fig. 4.2. Adaptive stepsize control of the both stiff integrators works satisfactorily: by the Rosenbrock stiff integrator the state of the isostatic equilibrium has been reached within 20 time steps, and the time instant of $10^6$ yr within 30 time steps. The speed of the integration is governed by the number of spatial grid points. Due to the band-diagonal structure of the underlying algebraic equations, the dependence of both the processor time and the allocated memory is a linear function of the number of spatial grid points. As an example
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Fig. 4.3. Surface Love numbers $h_2$, $l_2$ and $k_2$ of the homogeneous compressible model (symbols ♦) by the Rosenbrock stiff integrator. The response of the homogeneous incompressible model is shown, too (symbols +). Actually, the same as Fig. 8.1.

we can say that the Pentium/350 processor generates 20 time steps per second with 101 spatial grid points. For $n \leq 6$, even the grid of 11 equidistant points reveals satisfactory $h_n$ and $k_n$; for higher $n$, similar savings could be achieved by redistributing the grid points towards the surface. Actually, this is the case of 101 grid points for $n \geq 120$, too. Time steps produced by the both stiff integrators exhibit even distribution in the logarithmic scale. The Rosenbrook stiff integrator yields denser time-stepping which is rather universal: the Rosenbrook method by stiff utilizes just four intermediate functional evaluations per step, while the number of internal stages (i.e., the steps by $h$) per step (i.e., the step by $H$, cf. p. 39) employed by the semi-implicit extrapolation method by stiffbs is, in general, higher. The results from the interior points can not, unfortunately, be consistently employed due to the extrapolating character of the latter method. Let us remind that the expected isostatic limits are known analytically (Wu & Peltier 1982),

$$\lim_{t \to \infty} h_n(t) = -\frac{2n+1}{3}, \quad \lim_{t \to \infty} k_n(t) = -1.$$ (4.41)

The long-time values of the surface Love numbers fit these values accurately.

The surface Love numbers of the compressible homogeneous model for $n = 2$ are shown in Fig. 4.3. We see the fast onset of the exponential-like instability of the all three Love numbers. This is the indication of the gravitational collapse of the compressible homogeneous spheres which is discussed in greater detail in Chapter 8; in particular, Fig. 8.1 and Table 8.2 may be confronted.

In Fig. 4.4 we demonstrate the relaxation of the incompressible model again. Now we monitor not only the surface values of $y_J(t)$, but the depth dependence of the whole $y(t)$. The time evolution of the physical components of $y(t)$ has been plotted in the “one time step—one curve” manner. We meet a credible shape of the plotted curves with the amplitudes moving towards the surface with increasing $n$. We may also confirm the general acceptability of the boundary condition $y_0(t) = 0$, as has been announced above; in particular, the stress components $T_{rr,2}$ and $T_{r\theta,2}$ are the only non-zero components at $r = 0$.

The small number of time steps per degree required in order to obtain the response within the first $10^6$ yr appears to be the promising feature of the numerical implementation of the IV/MOL approach. However, other numerical features of the presented code must still be understood. In Fig. 4.5 we present the same content as in Fig. 4.1, now for the time interval of $10^{18}$ yr. We see the tendency of the horizontal Love numbers $l_n(t)$ to move away from the values reached within...
Fig. 4.4. Time evolution of the physical components of the discretized solution vector $y(t)$ of the homogeneous incompressible model from the elastic response at $t = 0$ up to $t = 10^6$ yr. The direction of the progress in time is depicted by the arrows; timing of the particular time instants can be revealed by comparison with the surface values given in Fig. 4.1. Spatial dimension of 6371 km has been discretized by 101 grid points. Vertical labelling is relative and has been suppressed.
Fig. 4.5. Time evolution of the surface Love numbers $h_n$, $l_n$ and $k_n$ of the homogeneous incompressible model evaluated by the IV/MOL approach. Similar to Fig. 4.1, but the time period of $10^{18}$ yr is shown. Various densities of the spatial discretization are considered: 11, 21, 101, 201 and 1001 grid points. See the text for the discussion (but not for the explanation) of the behaviour of $l_n(t)$.

the first $10^6$ yr. The time of the onset of this transition to other, somehow arbitrary, but constant values depends on the density of the spatial discretization; the higher density, the latter onset. In Fig. 4.6 we reveal the depth-dependence of the physical components of $y(t)$ that we have obtained for 101 equidistant grid points. Some of the computed field variables undergo a kind of overturning within the time scale of $10^6$–$10^{12}$ yr. This holds a sign of a numerically dependent effect, sensitive not to the choice of the stiff integrator or its internal parameters, but rather to the spatial-grid distribution. At the present moment we do not have a satisfactory explanation of this behaviour on hand. Note, however, that at the limit of $t \to \infty$, from the viewpoint of the NM approach, $V_n$ ought to become undefined.

The generalization of the tested code to process arbitrarily stratified 1-D models will require (i) preparation of appropriate values of $P$, $Q$ and $q$, (ii) evaluation of the initial elastic solution vector $y(0)$, and (iii) implementation of proper boundary conditions at the core-mantle boundary.

A report on the further development is postponed for a future work$^5$.

$^5$Ph.D. thesis is considered to be a limited project, and a finite amount of time should only be spent with its preparation (A. van den Berg, personal communication).
Fig. 4.6. Time evolution of the physical components of the discretized solution vector $y(t)$ of the homogeneous incompressible model from the elastic response at $t = 0$ to $t = 10^{12}$ yr. The direction of the progress in time is depicted by the arrows; the left arrows direct the evolution of the appropriate field variable for $t \leq 10^6$ yr (identical with Fig. 4.4), the right arrows show the progress during the overturning. No temporal development of the field variable for $t > 10^6$ yr is denoted by the symbol $\otimes$. 

radius $r$ [km]
4.6 Conclusion to Part I

We have finalized the formulation of the initial-value approach via the method of lines. The field partial differential equations (2.13)–(2.14) in the material-local form have been subjected to the spectral harmonic decomposition. With the elastic constitutive relation (2.10) being considered first, the procedure of derivation of the boundary-value problem for the ordinary differential equations (2.49) with respect to the radius has been exposed. The similar procedure, generalized for the Maxwell viscoelastic constitutive relation (2.15), has been introduced to derive the partial differential equations (3.23) with respect to both time and the radius. Similar differential systems, (3.56) and (3.104), respectively, have been derived with the constitutive relation of the standard linear solid and for the axially symmetric viscosity distribution. The partial differential equations (3.23) for the Maxwell solid have been further elaborated. In accordance with the idea of the method of lines, the spatial semi-discretization has been enforced. This has led to the ordinary differential equations (4.14) with respect to time in the form appropriate for the application of stiff integrators. We have adapted the Rosenbrock and the semi-implicit extrapolation stiff integrators, (4.31) and (4.33), respectively, to exploit the band-diagonal structure of the underlying linear differential equations. The efficiency of the derived formulation has been examined on the analytically tractable relaxation of the homogeneous, Maxwell viscoelastic sphere.

Another formulation of the IV approach has been derived from the partial differential equations (2.13)–(2.15) via the alternative semi-discretizing method of Rothe in Section 4.4. It is this formulation which has been employed in our published papers on the initial-value approach, collected in the following Part II.

\[ \text{ANTONÍN DVOŘÁK, Slavonic Dances, Op. 46. No. 4 in F major. Tempo di Minuetto (1878)} \]