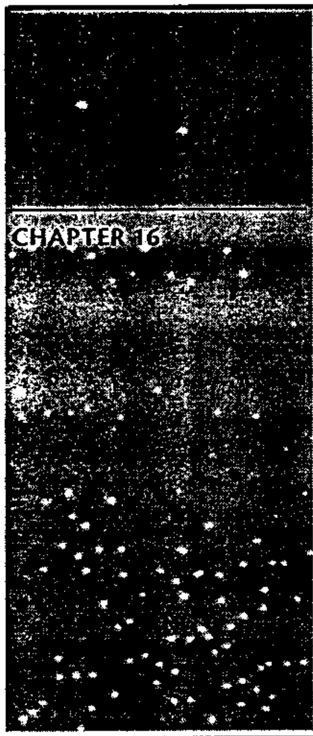

Time Integration of the Space Time Kinetics Equations

IN THIS CHAPTER, we will explore some of the techniques used in practice to integrate in time the equations of space-time kinetics. We have seen in the previous chapter how the spatial integration leads to the semi-discrete formulation of these equations. Also, even though we have used mesh centered finite differences, the techniques described here could be applied without change to other discretisations, such as nodal methods for example.

Theta Method

The semi-discrete form of the space-time kinetics equations (116) are the starting point of this analysis. The structure of the $[H]$ is also detailed on Figure 10, page 185. In this section, in order to simplify matters, we will only deal with the case where a single family of delayed precursors is modeled. Generalization to more families is straightforward.

We can write the matrix form in the following fashion,

$$\frac{d}{dt}\begin{bmatrix}\phi \\ C\end{bmatrix} = \begin{bmatrix}[H]_{11} & [H]_{12} \\ [H]_{21} & [H]_{22}\end{bmatrix}\begin{bmatrix}\phi \\ C\end{bmatrix}$$

We apply the Θ method to this equation, using a different value of Θ for the fluxes and for the precursors. We chose a formulation in which the Θ^P and the Θ^D are independent of space, but can be different from each other. Recall from chapter 11, *Numerical Integration Techniques*, page 123, that we can include the implicit, the explicit and the Crank-Nicholson schemes just by changing the value of the Θ. We thus have

$$\begin{bmatrix} [\phi]^{n+1} \\ [C]^{n+1} \end{bmatrix} - \begin{bmatrix} [\phi]^{n} \\ [C]^{n} \end{bmatrix} =$$

$$\Delta t \begin{bmatrix} [H]_{11}^{n+1} & [H]_{12}^{n+1} \\ [H]_{21}^{n+1} & [H]_{22}^{n+1} \end{bmatrix} \left\{ \begin{bmatrix} [\Theta]^{P} & [0] \\ [0] & [\Theta]^{D} \end{bmatrix} \begin{bmatrix} [\phi]^{n+1} \\ [C]^{n+1} \end{bmatrix} + \begin{bmatrix} [I-\Theta]^{P} & [0] \\ [0] & [I-\Theta]^{D} \end{bmatrix} \begin{bmatrix} [\phi]^{n} \\ [C]^{n} \end{bmatrix} \right\}$$

Solving this last equation might seem difficult on first hand, because of the very large number of unknowns in the problem. It is however possible to eliminate the C^{n+1} from the flux equations.

To do this, we rewrite the preceding system in two parts, one for the fluxes and one for the precursor concentrations, noting that the H_{12} and the H_{22} do not depend on time, since they only involve the λ_i, the group velocities and the volumes. We get

$$\begin{aligned} \phi^{n+1} - \phi^{n} = {} & \left[\Delta t H_{11}^{n+1} \Theta^{P}\right] \phi^{n+1} + \Delta t \left[H_{12}\right]\left[\Theta^{d}\right] C^{n+1} \\ & + \left[\Delta t H_{11}^{n}\left[I - \Theta^{P}\right]\right] \phi^{n} + \Delta t\left[H_{12}\right]\left[I - \Theta^{d}\right] C^{n} \end{aligned} \quad \text{(EQ 117)}$$

$$C^{n+1} - C^{n} = \left[\Delta t H_{21}^{n+1}\Theta^{p}\right]\phi^{n+1} + \Delta t\left[H_{22}\right]\left[\Theta^{d}\right]C^{n+1} + \left[\Delta t H_{21}^{n}\left[I - \Theta^{p}\right]\right]\phi^{n} + \Delta t\left[H_{22}\right]\left[I - \Theta^{d}\right]C^{n}$$

We isolate C^{n+1} from this last equation to get

$$\begin{aligned} C^{n+1} = {} & \left[I - \Delta t H_{22}\Theta^{d}\right]^{-1}\left[I + \Delta t H_{22}(I - \Theta^{d})\right]C^{n} \\ & + \left[I - \Delta t H_{22}\Theta^{d}\right]^{-1}\left[\Delta t H_{21}^{n+1}\Theta^{p}\right]\phi^{n+1} \\ & + \left[I - \Delta t H_{22}\Theta^{d}\right]^{-1}\left[\Delta t H_{21}^{n}\left[I - \Theta^{p}\right]\right]\phi^{n} \end{aligned} \quad \text{(EQ 118)}$$

We then substitute this result in the flux equation (117),

$$\begin{aligned} \phi^{n+1} - \phi^{n} = {} & \left[\Delta t H_{11}^{n+1}\Theta^{p}\right]\phi^{n+1} + \\ & + \Delta t\left[H_{12}\right]\left[\Theta^{d}\right]\left\{ \begin{aligned} & \left[I - \Delta t H_{22}\Theta^{d}\right]^{-1}\left[I + \Delta t H_{22}(I - \Theta^{d})\right]C^{n} \\ & + \left[I - \Delta t H_{22}\Theta^{d}\right]^{-1}\left[\Delta t H_{21}^{n+1}\Theta^{p}\right]\phi^{n+1} \\ & + \left[I - \Delta t H_{22}\Theta^{d}\right]^{-1}\left[\Delta t H_{21}^{n}\left[I - \Theta^{p}\right]\right]\phi^{n} \end{aligned} \right\} \\ & + \left[\Delta t H_{11}^{n}\left[I - \Theta^{p}\right]\right]\phi^{n} + \Delta t\left[H_{12}\right]\left[I - \Theta^{d}\right]C^{n} \end{aligned}$$

and, regrouping terms together,

$$\left\{I - \Delta t H_{11}^{n+1}\Theta^p - \Delta t H_{12}\Theta^d\left[I - \Delta t H_{22}\Theta^d\right]^{-1}\left[\Delta t H_{21}^{n+1}\Theta^p\right]\right\}\phi^{n+1}$$

$$= \left\{I + \Delta t\left[H_{12}\right]\Theta^d\left\{\Delta t H_{11}^n\left[I - \Theta^p\right] + \left[I - \Delta t H_{22}\Theta^d\right]^{-1}\left[\Delta t H_{21}^n\left[I - \Theta^p\right]\right]\right\}\right\}\phi^n$$

$$+ \Delta t\left[H_{12}\right]\Theta^d\left[I - \Delta t H_{22}\Theta^d\right]^{-1}\left[I + \Delta t H_{22}(I - \Theta^d)\right] + \Delta t\left[H_{12}\right]\left[I - \Theta^d\right]C^n$$

We define the matrix

$$\left[A\right]^{n+1} = [I - \Delta t H_{11}^{n+1}\Theta^p - \Delta t H_{12}\Theta^d(I - \Delta t H_{22}\Theta^d)^{-1}\Delta t H_{21}^{n+1}\Theta^p]$$

and the vector

$$\left[S\right]^n = [I + \Delta t H_{12}^{n+1}\Theta^d(I - \Delta t H_{22}\Theta^d)^{-1}\Delta t H_{21}^n(I - \Theta^p) + \Delta t H_{11}^n(I - \Theta^p)][\phi]^n + (\Delta t H_{12}\Theta^d(I - \Delta t H_{22}\Theta^d)^{-1}(I + \Delta t H_{22}(I - \Theta^d)) + \Delta t H_{12}^n(I - \Theta^d))[C]^n$$

Finally, the flux equations can be put in the form

$$\left[A\right]^{(n+1)}\left[\Phi\right]^{(n+1)} = \left[S\right]^{(n)}$$

Note that evaluating the vector $\left[S\right]^{(n)}$ does not present any particular difficulties, since the matrix inversions appearing in it involve only diagonal matrices. Furthermore, this vector depends only on the flux vectors $\Phi^{(n)}$ and on the precursor vector C^n, evaluated at the previous time interval, and are therefore available for the computation.

Constructing the matrix $\left[A\right]^{(n+1)}$ does not present any difficulty either, since the inverses that appear in its expression involve only diagonal matrices. The matrix $\left[A\right]^{(n+1)}$ will have the same *structure* as H_{11}. It will be tri-diagonal for 1-D problems, penta-diagonal for 2-D problems, and hepta-diagonal for 3-D problems.

Consequently, the evaluation of the fluxes only need solving a problem involving these matrix structures. LU decomposition could be used in 1-D, whereas iterative methods such as Gauss-Seidel, SOR, CCSI, etc. would be used in 3-D. Methods such as ADI decomposition could also be used in such cases.

Once the fluxes ϕ^{n+1} have been calculated, the precursors C^{n+1} could be determined by slightly rearranging equation (118),

$$
\begin{aligned}
C^{n+1} &= \left[I - \Delta t H_{22}\Theta^d\right]^{-1}\left[\Delta t H_{21}^{n+1}\Theta^p\right]\phi^{n+1} \\
&\quad + \left[I - \Delta t H_{22}\Theta^d\right]^{-1}\left\{\begin{array}{l}\left[I + \Delta t H_{22}(I - \Theta^d)\right]C^n \\ \quad + \left[\Delta t H_{21}^n\left[I - \Theta^p\right]\right]\phi^n\end{array}\right\}
\end{aligned}
$$

Exponential Transforms

The fluxes vary quite fast during a transient.Many times, the time intervals must be of the order of 10^{-4} and even 10^{-5} seconds). There is thus much interest for any approaches that would lead to significant reduction of the time step. The quasistatic method is one of them, permitting longer intervals between the computation of the spatial solutions.

Another method is that of the exponential transform. This supposes that the fluxes and the precursors undergo quasi-exponential variations in time. The idea is to remove this exponential behavior, and to deal with variables that will vary much more slowly than the original ones. By way of consequence, a much longer time step could be used.

To show this, we introduce new variables, η and ζ, related to the fluxes and to the precursor concentrations by the transformations

$$\begin{aligned} [\Phi] &= \exp\left(\left[\Omega^{p}\right]t\right)[\eta] \\ \left[C_e\right] &= \exp\left(\left[\Omega_e^{d}\right]t\right)\left[\zeta_e\right] \end{aligned} \qquad \text{(EQ 119)}$$

These should vary more slowly than the initial variables. Note that the $\left[\Omega^{p}\right]$ and $\left[\Omega_e^{d}\right]$ are diagonal matrices, and that the exponential of these matrices are also diagonal matrices. We only have to find the differential equations governing $[\eta]$ and $\left[\zeta_e\right]$. To do so, we start from the system

$$\frac{\partial}{\partial t}[\psi] = [H][\psi]$$

in which we substitute (119),

$$\frac{\partial}{\partial t}\begin{bmatrix}\Phi\\ C\end{bmatrix} = \begin{bmatrix}[H]_{11} & [H]_{12}\\ [H]_{21} & [H]_{22}\end{bmatrix}\begin{bmatrix}\Phi\\ C\end{bmatrix}$$

$$\frac{\partial}{\partial t}\begin{bmatrix}\exp([\Omega^p]t) & [0]\\ [0] & \exp([\Omega_e^d]t)\end{bmatrix}\begin{bmatrix}[\eta]\\ [\zeta_e]\end{bmatrix} = \begin{bmatrix}[H]_{11} & [H]_{12}\\ [H]_{21} & [H]_{22}\end{bmatrix}\begin{bmatrix}\exp([\Omega^p]t) & [0]\\ [0] & \exp([\Omega_e^d]t)\end{bmatrix}\begin{bmatrix}[\eta]\\ [\zeta_e]\end{bmatrix}$$

The left hand side of this last equation can be written

$$\begin{bmatrix}\exp([\Omega^p]t)[\Omega^p] & [0]\\ [0] & \exp([\Omega_e^d]t)[\Omega_e^d]\end{bmatrix}\begin{bmatrix}[\eta]\\ [\zeta_e]\end{bmatrix} + \begin{bmatrix}\exp([\Omega^p]t) & [0]\\ [0] & \exp([\Omega_e^d]t)\end{bmatrix}\frac{\partial}{\partial t}\begin{bmatrix}[\eta]\\ [\zeta_e]\end{bmatrix}$$

so that

$$\begin{bmatrix}\exp([\Omega^p]t) & [0]\\ [0] & \exp([\Omega_e^d]t)\end{bmatrix}\frac{\partial}{\partial t}\begin{bmatrix}[\eta]\\ [\zeta_e]\end{bmatrix}$$
$$= \begin{bmatrix}[H]_{11} - \exp([\Omega^p]t)[\Omega^p] & [H]_{12}\\ [H]_{21} & [H]_{22} - \exp([\Omega_e^d]t)[\Omega_e^d]\end{bmatrix}\begin{bmatrix}[\eta]\\ [\zeta_e]\end{bmatrix}$$

Multiplying by the inverse of the matrix exponential

$$\frac{\partial}{\partial t}\begin{bmatrix}[\eta]\\ [\zeta_e]\end{bmatrix} = \begin{bmatrix}\exp\left(-[\Omega^p]t\right)[H]_{11}-[\Omega^p] & \exp\left(-[\Omega^p]t\right)[H]_{12}\\ \exp\left(-[\Omega_e^d]t\right)[H]_{21} & \exp\left(-[\Omega_e^d]t\right)[H]_{22}-[\Omega_e^d]\end{bmatrix}\begin{bmatrix}[\eta]\\ [\zeta_e]\end{bmatrix} \tag{EQ 120}$$

We can rewrite this last system in the form

$$\frac{\partial}{\partial t}\begin{bmatrix}\eta\\ \zeta\end{bmatrix} = [H']\begin{bmatrix}\eta\\ \zeta\end{bmatrix}$$

The elements of matrix $[H']$ are obtained from the expressions found in equation (120). Since we have a system having the same structure as the initial system, the methods introduced in the previous section can be used to perform the temporal integration.

Frequency Determination

There is a problem to be addressed, that of the way to determine the frequencies $[\Omega^p]$ and $[\Omega_e^d]$. The temporal behavior of the fluxes and the precursors is not exactly an exponential during most of complex transients. There is therefore no frequencies that will permit following the fluxes exactly during a given time interval.

Approximate methods to determine the frequencies thus have to be sought. A simple and often used technique is to calculate the frequencies for the time interval $t_n < t < t_{n+1}$ in the following way,

$$\Omega^{p}_{g,\,ijk} = \frac{1}{\Delta t}\log\left(\frac{\phi^{n}_{g,\,ijk}}{\phi^{n-1}_{g,\,ijk}}\right)$$

and

$$\Omega^{d}_{e,\,ijk} = \frac{1}{\Delta t}\log\left(\frac{C^{n}_{e,\,ijk}}{C^{n-1}_{e,\,ijk}}\right)$$

This is to suppose that the frequencies used in a given time interval are those that were present in the preceding time interval. This approximation works relatively well, except when reactivity devices move in discontinuous fashion, for example when they start or stop moving. In such circumstances, the calculated frequencies will not be very good, and smaller time steps will be necessary.