CHAPTER 11

Numerical Integration Techniques

EXACT SOLUTIONS of the point kinetics equations present many difficulties, as we have seen in the previous chapter. Thus we look at approximate integration methods. A complete numerical analysis course could be written on them. We will examine a very small number of them, and then only from a practical point of view, and letting go of much mathematical rigor.

Criteria

In practice, the choice of a numerical method relies on 3 main criteria,

- truncation error
- stability
- ease of computation

Equilibrium between these 3 criteria will vary from analysis to analysis. In some cases, stability of the solution might be overpowering, in other cases ease of computation might be more important.

We will only look at integration methods that are easily generalized for the space discretized equations. Therefore, the Runge-Kutta methods and the predictor-corrector methods will not be discussed here, because the methods are not very well adapted to the space-time kinetics methods.

In order to review each of the 3 criteria for a few very simple methods, we rewrite here the point kinetics equations in the form

$$\frac{d}{dt}\Psi = R\Psi \qquad \text{(EQ 84)}$$

In this chapter, we will use the following notation:

- $\Delta t = t_{n+1} - t_n$
- $\Psi^n \equiv \Psi(t_n)$

Also, in the stability evaluation, we will suppose that the operator R stays constant during a given transient.

We will use the principle, without proving it, that the stability properties of a numerical scheme does not depend on the particular choice of basis used to represent vectors and matrices involved in the problem.

We will consider three numerical schemes, the explicit method, the implicit method and the Crank-Nicholson method. We will then see that the Θ method integrates these three methods into one.

The first step, for all the methods that we will analyze is to replace the time derivative in (84) by

$$\frac{d}{dt}\Psi \approx \frac{\Psi^{n+1} - \Psi^{n}}{\Delta t}$$

Explicit Method

In the explicit method, the right hand side of (84) is replaced by $R\Psi^{n}$. In this case, (84) becomes

$$\Psi^{n+1} = (I + R\Delta t)\Psi^{n} \qquad \text{(EQ 85)}$$

Truncation Error

Formally, the exact solution of the differential equation (84)is an exponential of the matrix R, which is

$$\Psi^{n+1} = \exp(R\Delta t)\Psi^{n}$$

The truncation error is the difference between are approximate solution and the exact solution of the differential equation. Consequently, the truncation error ET will be given by

$$\begin{aligned} ET &= (I + R\Delta t)\Psi^n - \exp(R\Delta t)\Psi^n \\ &= (I + R\Delta t - \exp R\Delta t)\Psi^n \end{aligned}$$

Let us now perform the expansion of the matrix exponential,

$$ET = \left(I + R\Delta t - \left(I + R\Delta t + \frac{1}{2}R^2\Delta t^2 + \ldots\right)\right)\Psi^n$$

and consequently

$$ET \approx -\frac{1}{2}R^2\Delta t^2\Psi^n$$

The explicit method is thus of order $\frac{1}{2}\Delta t^2$.

Stability

In order to examine stability, we first express our differential equation in the basis that diagonalizes the matrix R. In this case, we go back to equation (85) that we rewrite in the particular basis

$$x^{n+1} = (1 + \omega\Delta t)x^n$$

The ω will thus be eigenvalues of R, in other words, the roots of Nordheim's equation (83).

If we start from the initial conditions x^0 at time $t = 0$, the first cycle of calculations will bring up a vector x^1,

$$x^1 = (1 + \omega\Delta t)x^0$$

The second cycle applied to x^1 will bring

$$x^2 = (1 + \omega\Delta t)x^1$$

Thus

$$\begin{aligned} x^2 &= (1 + \omega\Delta t)(1 + \omega\Delta t)x^0 \\ &= (1 + \omega\Delta t)^2 x^0 \end{aligned}$$

Continuing this process, we find

$$x^{n+1} = (1 + \omega\Delta t)^{n+1} x^0$$

If for example we had a negative reactivity, we know that all the roots ω are negative, and we must have a solution that decreases in time. Consequently

$$|1 + \omega\Delta t| < 1$$

must hold. This can also be written as

$$-1 < 1 + \omega\Delta t < 1$$

Let us now replace ω by $-|\omega|$ to emphasize that all ω are negative,

$$-1 < 1 - |\omega|\Delta t < 1$$

The system will be stable if both branches of the inequality are true. Two possibilities must be examined: $1 - |\omega|\Delta t < 1$ and $-1 < 1 - |\omega|\Delta t$.

- Case 1 : $1 - |\omega| \Delta t < 1$

  We substract 1 from each side of this inequality, to get $-|\omega| \Delta t < 0$. This is always true.

- Case 2 : $-1 < 1 - |\omega| \Delta t$

  We substract 1 from each side of this inequality, to get $-2 < -|\omega| \Delta t$. We change the sign by multiplying by -1 and we reverse the sides of the inequality,

$$|\omega| \Delta t < 2$$

or

$$\Delta t < \frac{2}{|\omega|} \tag{EQ 86}$$

There is thus a condition on Δt in order to insure stability of the explicit scheme. This stability condition (86) is very restrictive. The negative roots of Nordheim's equations are very negative, and the most negative of them is smaller than $-\lambda_D$, being around $-\frac{\beta}{\Lambda}$. Therefore, time steps smaller than 10 to 20 milli-seconds will be necessary, otherwise spurious oscillations of fast increasing amplitudes will overtake the solution.

Ease of computation

The explicit method, given in (85) involves only the multiplication of a matrix by a vector to obtain the solution at the next time step. From this point of view, the explicit method is very simple, and is very easy to implement. It will not necessitate very large computing resources.

Implicit Method

Our approach will be the same as that of the explicit method. In the implicit scheme, we replace the right hand side of (84) by $R\Psi^{n+1}$, instead of the $R\Psi^{n}$ of the explicit method. The implicit method is thus

$$\frac{\Psi^{n+1} - \Psi^{n}}{\Delta t} = R\Psi^{n+1} \qquad \text{(EQ 87)}$$

We regroup the terms in Ψ^{n+1} and in Ψ^{n} to get

$$(I - R\Delta t)\Psi^{n+1} = \Psi^{n}$$

and we express Ψ^{n+1} in terms of Ψ^{n},

$$\Psi^{n+1} = (I - R\Delta t)^{-1}\Psi^{n}$$

Truncation Error

The truncation error is obtained by the difference between the approximate solution and the exact solution,

$$ET = (I - R\Delta t)^{-1}\Psi^{n} - \exp(R\Delta t)\Psi^{n}$$

and if we make the expansions

$$ET = (I + R\Delta t + R^2\Delta t^2 + \ldots)\Psi^{n} - \left(I + R\Delta t + \frac{1}{2}R^2\Delta t^2 + \ldots\right)\Psi^{n}$$

which gives

$$ET = \frac{1}{2}R^2\Delta t^2\Psi^n$$

Consequently, the implicit method is a method of order $\frac{1}{2}\Delta t^2$. The coefficient of Δt^2 is ½, the same as that of the explicit method.

Stability

Again, we express the system in the vector basis that diagonalizes it.If we examine the sequence of solution vectors, we have

$$\begin{aligned}
x^1 &= (1-\omega\Delta t)^{-1}x^0 \\
x^2 &= (1-\omega\Delta t)^{-1}x^1 \\
&= (1-\omega\Delta t)^{-1}(1-\omega\Delta t)^{-1}x^0 \\
&= (1-\omega\Delta t)^{-2}x^0 \\
&\cdot \\
x^{n+1} &= (1-\omega\Delta t)^{-(n+1)}x^0
\end{aligned}$$

Consequently, we will have a stable solution if

$$-1 < \frac{1}{1-\omega\Delta t} < 1$$

We must have a solution that goes to 0 when reactivity is negative, that is when all the ω are negative. In this case, ω can be replaced by $-|\omega|$, which gives

$$-1 < \frac{1}{1+|\omega|\Delta t} < 1$$

Since $1 + |\omega|\Delta t$ is positive, we can multiply the inequality by this factor without changing the inequalities themselves

$$-(1 + |\omega|\Delta t) < 1 < (1 + |\omega|\Delta t)$$

We examine each of these in turn:

- Case 1 $-(1 + |\omega|\Delta t) < 1$:

  We have that $1 + |\omega|\Delta t$ is always greater than 1, since $|\omega|$ is always positive. Consequently, the left hand side is always negative, and thus always smaller than 1. The inequality is always true.

- Case 2 $1 < (1 + |\omega|\Delta t)$:

  Substracting 1 from each side of the inequality, which gives $0 < |\omega|\Delta t$. But the value of $|\omega|$ is always positive. Then the inequality is always true.

The stability conditions are thus always satisfied. We conclude that the implicit method is unconditionally stable.

Ease of Computation

The implicit method, given in (87) requires the inversion of the matrix R to get the solution at the next time step. This matrix can change at each time interval, according to the cross-section and reactivity changes. The inversion will have to be performed at each time interval. From this point of view, the implicit method requires more calculation effort and time than the explicit method. It has the advantage of unconditional stability, but at the cost of a matrix inversion.

Crank-Nicholson Method

Again we follow our previous approach. In the Crank-Nicholson scheme, we replace the right hand side of (84) by $\frac{1}{2}R\Psi^n + \frac{1}{2}R\Psi^{n+1}$, the average of the solution vectors taken at time t_n and at t_{n+1}. The Crank-Nicholson is then

$$\frac{\Psi^{n+1} - \Psi^n}{\Delta t} = \frac{1}{2}R\Psi^n + \frac{1}{2}R\Psi^{n+1} \qquad \text{(EQ 88)}$$

which becomes, after regrouping the vectors belonging to identical times,

$$\left(I - \frac{1}{2}R\Delta t\right)\Psi^{n+1} = \left(I + \frac{1}{2}R\Delta t\right)\Psi^n$$

and isolating the new solution vector in terms of the previous vector

$$\Psi^{n+1} = \left(I - \frac{1}{2}R\Delta t\right)^{-1}\left(I + \frac{1}{2}R\Delta t\right)\Psi^n$$

Truncation Error

Once again, the truncation is obtained by the difference between the approximate solution and the exact solution, which becomes in the Crank-Nicholson scheme

$$ET = \left(I - \frac{1}{2}R\Delta t\right)^{-1}\left(I + \frac{1}{2}R\Delta t\right)\Psi^n - \exp(R\Delta t)\Psi^n$$

Performing the expansion

$$\left(I - \frac{R\Delta t}{2}\right)^{-1}\left(I + \frac{R\Delta t}{2}\right) = \left(I + \frac{1}{2}R\Delta t + \left(\frac{1}{2}R\Delta t\right)^2 + \ldots\right)\left(I + \frac{R\Delta t}{2}\right)$$

$$= I + 2\frac{1}{2}R\Delta t + 2\left(\frac{1}{2}R\Delta t\right)^2 + 2\left(\frac{1}{2}R\Delta t\right)^3 + \ldots$$

Together with the expansion of the matrix exponential, the truncation error can be expressed as

$$ET = \left(I + R\Delta t + \frac{1}{2}(R\Delta t)^2 + \frac{1}{4}(R\Delta t)^3 + \ldots\right)$$
$$-\left(I + R\Delta t + \frac{1}{2}R^2\Delta t^2 + \frac{1}{6}R^3\Delta t^3 + \ldots\right)$$

Stopping the expansions to terms in Δt^3 gives

$$ET = \frac{1}{12}R^3\Delta t^3$$

Therefore, the Crank-Nicholson method is of order $\frac{1}{12}\Delta t^3$.

Stability

Here also we change the basis in which the matrix is expressed to one in which it is diagonal. Examining the series of solution vectors shows that

$$x^1 = \left(1 - \frac{\omega\Delta t}{2}\right)^{-1}\left(1 + \frac{\omega\Delta t}{2}\right)^1 x^0$$

$$x^2 = \left(1 - \frac{\omega\Delta t}{2}\right)^{-1}\left(1 + \frac{\omega\Delta t}{2}\right)^{1} x^1$$

$$= \left(1 - \frac{\omega\Delta t}{2}\right)^{-2}\left(1 + \frac{\omega\Delta t}{2}\right)^{2} x^0$$

.

$$x^{n+1} = \left(1 - \frac{\omega\Delta t}{2}\right)^{-(n+1)}\left(1 + \frac{\omega\Delta t}{2}\right)^{n+1} x^0$$

$$= \left(\frac{1 + \frac{\omega\Delta t}{2}}{1 - \frac{\omega\Delta t}{2}}\right)^{n+1} x^0$$

The solution will be stable if

$$-1 < \left(\frac{1 + \frac{\omega\Delta t}{2}}{1 - \frac{\omega\Delta t}{2}}\right) < 1$$

We must have a solution that tends to 0 when reactivity is negative, that is when all the ω are negative.

In such a case, ω can be replaced by $-|\omega|$, and we find for the stability conditions

$$-1 < \left(\frac{1 - \frac{|\omega|\Delta t}{2}}{1 + \frac{|\omega|\Delta t}{2}}\right) < 1$$

since the denominator is always positive, it can multiply the two inequalities without affecting the inequality signs, which gives

$$-\left(1+\frac{|\omega|\Delta t}{2}\right)<1-\frac{|\omega|\Delta t}{2}<\left(1+\frac{|\omega|\Delta t}{2}\right)$$

We only have to examine each of these to find the stability conditions

- Case 1 $1-\frac{|\omega|\Delta t}{2}<\left(1+\frac{|\omega|\Delta t}{2}\right)$:

  Add $|\omega|\Delta t/2$ on each side of the inequality, to get
  $1<1+|\omega|\Delta t$ which of course is always true.
- Case 2 $-(1+|\omega|\Delta t/2)<1-|\omega|\Delta t/2$: Substract 1 from each side, and get $-2-|\omega|\Delta t/2<-|\omega|\Delta t/2$ which is also always true.

The Crank-Nicholson method is therefore unconditionally stable.

Ease of Computation

The Crank-Nicholson method (88) requires the multiplication of a vector by a matrix followed by a matrix inversion and another matrix multiplication. The method is thus somewhat expensive in computer resources. However, the matrix-vector multiplication is not very demanding compared to the matrix inversion. The Crank-Nicholson method is barely more expensive than the implicit method.

Theta Method

This method is a generalization of the type of methods that we just examined. It consists in discretizing system (84) in the following way:

$$\frac{\Psi^{n+1} - \Psi^{n}}{\Delta t} = (1 - \Theta)R\Psi^{n} + \Theta R\Psi^{n+1} \qquad \text{(EQ 89)}$$

In other words, the right hand side is a linear combination of the vectors taken at time t_n and t_{n+1}. Regrouping the vectors belonging to the same time,

$$\begin{aligned}(I - \Theta R\Delta t)\Psi^{n+1} &= (I + (1 - \Theta))R\Delta t\Psi^{n} \\ \therefore \Psi^{n+1} &= (I - \Theta R\Delta t)^{-1}(I + (1 - \Theta))R\Delta t\Psi^{n}\end{aligned}$$

We find immediately that

- $\Theta = 0$ gives the explicit method
- $\Theta = 1/2$ gives the Crank-Nicholson method
- $\Theta = 1$ gives the implicit method

So the Θ method will require the same resources as that of the Crank-Nicholson method. Also, with a fixed Δt, both implicit and explicit methods can also be reproduced.

The main advantage of this method is the possibility to vary the value of Θ during a transient. This could then give the best possible method as a function of observed variations of the solution during the transient.