Solution: HW3

ME526/NSE526

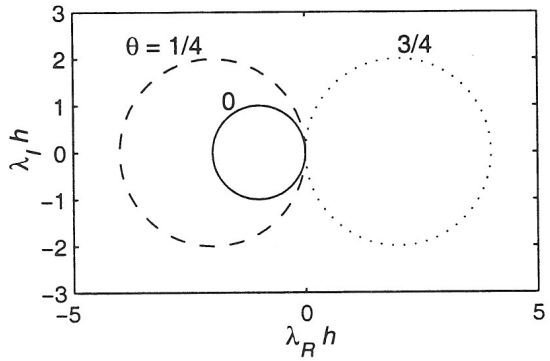
1. Model problem for $y' = f(y,t)$ is $y' = \lambda y = (\lambda_R + i\lambda_I)y$. For the scheme given, the amplification factor is given as

$$\sigma = y_{n+1}/y_n = \frac{1+\lambda h(1-\theta)}{1-\lambda h\theta}. \tag{1}$$

Setting $\sigma \leq 1$ for the limiting stability condition ($\sigma = 1$), we get

$$(\lambda_R h - \frac{1}{2\theta-1})^2 + (\lambda_I h)^2 = \frac{1}{(2\theta-1)^2}, \tag{2}$$

which is a circle of center $(\frac{1}{2\theta-1}, 0)$ and radius $\frac{1}{|2\theta-1|}$. For $0 \leq \theta \leq 0.5$, the circle is in the left side of the complex plane and the region of stability is inside the circle. For $0.5 \leq \theta \leq 1$, the circle is on the right side and the region of stability is *outside* the circle for $\lambda_R < 1$.



2. Applying the scheme to $y' = \lambda y$ one gets

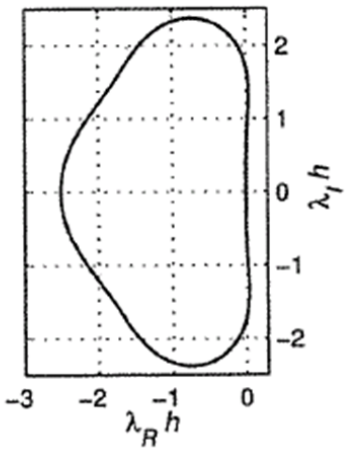
$$y_{n+1} = y_n(1 + \lambda h + \frac{1}{2}\lambda^2 h^2 + \frac{1}{6}\lambda^3 h^3) \tag{3}$$

This is a globally third order accurate scheme. It is similar to the third order schem RK3.

$$\begin{aligned} y^* &= y_n + \gamma_1 h\lambda y_n = y_n(1+\gamma_1\lambda h) \\ y^{**} &= (y_n + \gamma_1 h\lambda y_n) + \gamma_2 h\lambda(y_n + \gamma_1 h\lambda y_n) + \omega_2 h\lambda y_n \\ &= y_n(1 + \gamma_1\lambda h + \gamma_2\lambda h + \gamma_2\gamma_1 h^2\lambda^2 + \omega_2\lambda h) \\ &= y_n(1 + (\gamma_1 + \gamma_2 + \omega_2)\lambda h + \gamma_2\lambda^2 h^2) \end{aligned}$$

$$
\begin{aligned}
y_{n+1} &= y^{**} + \gamma_3 h\lambda y^{**} + \omega_3 h\lambda y^{*} \\
&= y^{**}(1 + \gamma_3 h\lambda) + \omega_3 h\lambda y^{*} \\
&= y_n[(1 + (\gamma_1 + \gamma_2 + \omega_2)\lambda h + \gamma_2\lambda^2 h^2)](1 + \gamma_3 h\lambda) + \omega_3 h\lambda(1 + \gamma_1 h\lambda)y_n \\
&= y_n[(1 + (\gamma_1 + \gamma_2 + \omega_2)\lambda h + \gamma_2\lambda^2 h^2)(1 + \gamma_3 h\lambda) + \omega_3 h\lambda(1 + \gamma_1 h\lambda)]
\end{aligned}
$$

Simplify to show that you get the above expression, which is same as the Taylor series expansion for the first four terms. This is third-order accurate globally.



3. The analytical steady state solution is obtained by setting the time rates of change of species concentrations to zero. This gives $C_1 = 0$, $C_2 = 0$, and $C_3 = 1$.

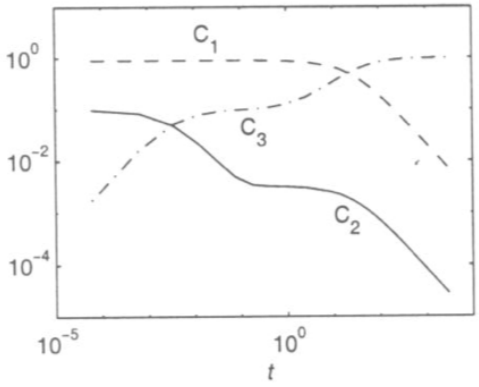
   The Jacobian matrix (obtained after linearization about t_n) at t_n is:

$$
A_n = \begin{bmatrix} -k_1 & k_2 C_3 & k_2 C_2 \\ k_1 & -k_2 C_3 - 4k_3 C_2 & -k_2 C_2 \\ 0 & 4k_3 C_2 & 0 \end{bmatrix} \tag{4}
$$

   where the concentrations C_i in the above matrix equation are evaluated at t_n and thus are known. The eigenvalues of the matrix at $t = 0$ are: 0, -1.0417, and -598.9983. We clearly see that $|\lambda_{max}/\lambda_{min}| >> 1$, and hence the problem is stiff. The eigenvalues are real and negative. The estimate for the maximum time-step for $RK4$ scheme based on its stability curve is $\Delta t = 2.79/598.9983 = 0.0047$. Note that in general the time-step requirement will vary as we integrate the solution in time, because the eigenvalues of the matrix may change. For this problem, one can show that the initial condition based eigenvalues are most restrictive. Using a time step of $\Delta t = 0.003$ as a fixed one, it is easy to see that the

solution would take $3000/0.003 \approx 10^6$ steps! Huge computational effort. Depending upon what machine you use this may take up to hrs!

Using the stifbs (ODE solver), only 28 steps were required for an error tolerance of 10^{-9}, a significant saving in computing time. The solutions obtained from the two schemes are very similar:



Central Differencing gives,

$$\mathbf{C}^{n+1} = \mathbf{C}^n + \frac{\Delta t}{2}\left[\underbrace{\mathbf{F}(\mathbf{C}^{n+1})}_{\text{linearize}} + \mathbf{F}(\mathbf{C}^n)\right] \tag{5}$$

Since $[\mathbf{F}(\mathbf{C}^{n+1})$ is a non-linear function of C_1, C_2, and C_3 at time t_{n+1}, we need to linearize it using Taylor Series expansion around t_n.

$$\mathbf{F}(\mathbf{C}^{n+1}) = \mathbf{F}(\mathbf{C}^n) + \underbrace{\left.\frac{\partial \mathbf{F}}{\partial \mathbf{C}}\right|_{t_n}}_{\text{Jacobian=A}_\text{n}} \left(\mathbf{C}^{n+1} - \mathbf{C}^n\right) + \text{higher order terms} \tag{6}$$

$$\approx \mathbf{F}(\mathbf{C}^n) + A_n\left(\mathbf{C}^{n+1} - \mathbf{C}^n\right) \tag{7}$$

Substitute for $\mathbf{F}(\mathbf{C}^{n+1})$ in the above equation and simplify to get

$$\mathbf{C}^{n+1} = \mathbf{C}^n + \frac{\Delta t}{2}\left[\underline{\mathbf{F}(\mathbf{C}^n)} + A_n\left(\mathbf{C}^{n+1} - \mathbf{C}^n\right) + \underline{\mathbf{F}(\mathbf{C}^n)}\right] \tag{8}$$

$$\therefore \mathbf{C}^{n+1} = \left(\mathbf{C}^n - \frac{\Delta t}{2}A_n\mathbf{C}^n\right) + \frac{\Delta t}{2}A_n\mathbf{C}^{n+1} + \Delta t\mathbf{F}(\mathbf{C}^n) \tag{9}$$

$$\therefore \underbrace{\left(I - \frac{\Delta t}{2}A_n\right)}_{\mathbf{B}}\underbrace{\mathbf{C}^{n+1}}_{\bar{Y}} = \underbrace{\left(I - \frac{\Delta t}{2}A_n\right)}_{\mathbf{D}}\underbrace{\mathbf{C}^n}_{\bar{X}} + \underbrace{\Delta t\mathbf{F}(\mathbf{C}^n)}_{\bar{b}}. \tag{10}$$

It turns out that $\mathbf{B} = \mathbf{D}$. This linearized central scheme is easy to invert (finding inverse of B is easy, only a 3×3 matrix, original central will have non-linear terms that are not

easy to solve for). One does need to compute A_n at each time-step as it depends on the solution at t_n. Fewer time-steps would be needed to reach steady state as this method is unconditionally stable. The solution is also easier to obtain compared to true non-linear scheme. This method will still be second-order scheme compared to RK4 (fourth order), but one can use larger time-steps to reach the steady state. Owing to implicit nature of the scheme, even large time-steps will maintain stability in the transient regions and the stiffness problem is easily overcome as compared to the RK4 scheme.