## Homework XII

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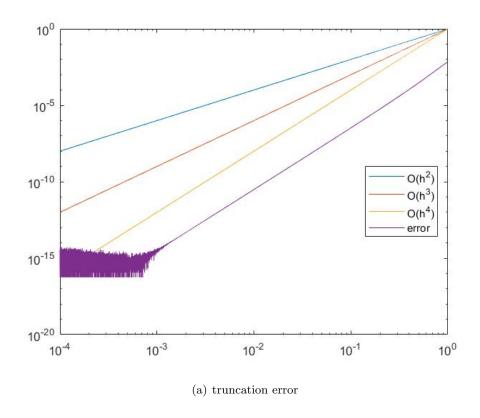
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## Abstract

This is Daniel's homework of "Numerical Algorithms with Case Studies II".

## 1 Problems

Q1 Implement the code and examine the truncation error of RK4 on loglog() plots.



Most of the truncation error satisfy  $O(h^4)$  level, while further accuracy cannot be reached because of rounding error.

**Q2** In this implicit method, we will have the following loop invariant in each iteration.

$$u_{k+1} = u_k + h(\theta f(t_k + h, u_{k+1}) + (1 - \theta)f(t_k, u_k))$$
(1)

$$= u_k - h\theta \lambda u_{k+1} - h(1-\theta)\lambda u_k \tag{2}$$

So after each iteration, we will have,

$$u_{k+1} = \frac{1 - h(1 - \theta)\lambda}{1 + h\theta\lambda} u_k \tag{3}$$

And to make  $u_k \to 0$  when  $k \to \infty$ , we have to let,

$$\frac{1 - h(1 - \theta)\lambda}{1 + h\theta\lambda} < 1\tag{4}$$

Which gives h > 0.

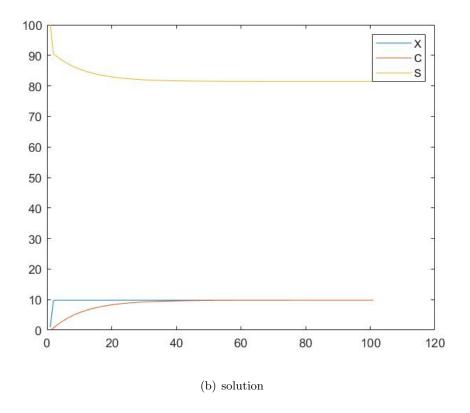
However, this is not sufficient for convergence, because we must take a good step h to make sure every implicit equation converges within each iteration. That gives the condition that  $x = (1 - h(1 - \theta)\lambda)y - h\theta\lambda x$  must converge.

$$||x_k + 1 - x_k|| = h\theta\lambda ||x_k - x_{k-1}|| \tag{5}$$

$$h < \frac{1}{\theta \lambda} \tag{6}$$

Therefore,  $h \in (0, \frac{1}{\theta \lambda})$ . However, numerical studies show that there could be an even tighter upper bound for stepsize.

Q3 The stationary concentrations are approximately X = 0.097754, C = 0.097749, S = 0.814495



 $\mathbf{Q4}$