HMTHCS 212 Assignment 3 Name ______________________

This assignment is due by **Monday July 18, 2022** by 6pm.

1. (10 points)

   (a) Find the values of the coefficients α, β, and γ and order of convergence p such that $f'(x)$ is best approximated by the formula

$$f'(x) = \frac{\alpha f(x+h) + \beta f(x) + \gamma f(x-2h)}{h} + \mathcal{O}(h^p)$$

Solution:

$$\alpha f(x+h) = \alpha \left[f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f^{(3)}(\xi_1) \right]$$

$$\beta f(x) = \beta f(x)$$

$$\gamma f(x-2h) = \gamma \left[f(x) - 2hf'(x) + \frac{(2h)^2}{2} f''(x) - \frac{(2h)^3}{6} f^{(3)}(\xi_2) \right].$$

Combining similar terms, we get

$$\begin{aligned} \alpha f(x+h) + \beta f(x) + \gamma f(x-2h) &= [\alpha + \beta + \gamma] f(x) \\ &+ [\alpha - 2\gamma] hf'(x) \\ &+ [\alpha + 4\gamma] \frac{h^2}{2} f''(x) \\ &+ \frac{h^3}{6} \left[\alpha f^{(3)}(\xi_1) - 8\gamma f^{(3)}(\xi_2) \right] \end{aligned}$$

where $\xi_1 \in (x, x+h)$ and $\xi_2 \in (x-2h, x)$ .We require that the coefficients satisfy the following conditions:

$$\begin{aligned} \alpha + \beta + \gamma &= 0 \\ \alpha - 2\gamma &= 1 \\ \alpha + 4\gamma &= 0 \end{aligned}$$

From the third equation

$$\alpha = -4\gamma$$

hence plugging into the second equation

$$-4\gamma - 2\gamma = 1$$

i.e.

$$\boxed{\gamma = -\frac{1}{6}, \quad \alpha = \frac{4}{6}, \quad \beta = -\frac{3}{6}}$$

The error term is then

$$\frac{h^3}{6}\left[\frac{4}{6}f^{(3)}(\xi_1)+\frac{8}{6}f^{(3)}(\xi_2)\right]=\frac{h^3}{6}\cdot 2\cdot f^{(3)}(\xi)=\frac{h^3}{3}f^{(3)}(\xi)$$

where $\xi \in (x-2h, x+h)$ where we have used the **Generalized Intermediate Value Theorem**:

There exists a $\xi \in (x-2h, x+h)$ such that for $g(x) = f^{(3)}(x)$ we have

$$g(\xi)=\frac{w_1 g(\xi_1)+\cdots+w_n g(\xi_n)}{w_1+\cdots+w_n}$$

with $n = 2$ and $w_1 = \frac{4}{6}$ and $w_2 = \frac{8}{6}$.

Hence

$$\boxed{f'(x)=\frac{4f(x+h)-3f(x)-f(x-2h)}{6h}-\frac{h^2}{3}f^{(3)}(\xi)}$$

(b) Using the formula derived from part (a), find an approximation of the derivative $f'(a)$ for the function $f(x) = \ln(x)$ at $a = 1$ for the following values of h (correct to 6 decimal places).

(i) $h = 0.1$

(ii) $h = 0.05$

(iii) $h = 0.025$

Solution:

$$\frac{4\ln(1+0.1)-3\ln(1)-\ln(1-0.2)}{0.6}=1.007307$$

$$\frac{4\ln(1+0.05)-3\ln(1)-\ln(1-0.1)}{0.3}=1.001737$$

$$\frac{4\ln(1+0.025)-3\ln(1)-\ln(1-0.05)}{0.15}=1.000425$$

(c) Compute the exact value of the derivative $f'(1)$ and then find the absolute errors of the approximations for each of the three values of h in part (b) (correct to 6 decimal places).

Solution:

The exact derivative is $f'(1) = 1$. The absolute errors are

$$|1-1.007307| = 0.007307$$

$$|1-1.001737| = 0.001737$$

$$|1-1.000425| = 0.000425$$

(d) Let E_h be the absolute error for the approximation of the derivative $f'(1)$ from part (c) for a value of h. By computing $E_{0.1}/E_{0.05}$ and $E_{0.05}/E_{0.025}$, comment on the order of convergence.

Solution:

$$E_{0.1}/E_{0.05} = \frac{0.007307}{0.001737} = 4.206$$
$$E_{0.05}/E_{0.025} = \frac{0.001737}{0.000425} = 4.088$$

We see that when the value of h is reduced by a factor of 2, then the error is reduced by a factor of 4. This shows that the rate of convergence is second order, that is $\mathcal{O}(h^2)$ as predicted by the error term.

2. (10 points)

(a) Find the values of the weights a_0, a_1 and a_2 such that the quadrature formula

$$\int_0^1 f(x)\,dx \approx a_0 f(0) + a_1 f(0.25) + a_2 f(1)$$

has the highest possible degree of precision.

Solution:

We want to find the highest degree of a monomial such that the quadrature formula gives an exact solution

$$\int_0^1 1\,dx = 1 = a_0 + a_1 + a_2$$

$$\int_0^1 x\,dx = \frac{1}{2} = \frac{1}{4}a_1 + a_2$$
$$\int_0^1 x^2\,dx = \frac{1}{3} = \frac{1}{16}a_1 + a_2$$

From the second equation,

$$a_2 = \frac{1}{2} - \frac{1}{4}a_1.$$

Substituting into the third equation

$$\frac{1}{3} = \frac{1}{16}a_1 + \frac{1}{2} - \frac{1}{4}a_1$$

So that

$$\frac{3}{16}a_1 = \frac{1}{6} \longrightarrow a_1 = \frac{16}{3}\cdot\frac{1}{6} = \frac{8}{9}$$

Hence

$$a_2 = \frac{1}{2} - \frac{1}{4}\frac{8}{9} = \frac{5}{18}.$$

Finally,

$$a_0 = 1 - \frac{8}{9} - \frac{5}{18} = 1 - \frac{7}{6} = -\frac{1}{6}$$

Hence,

$$\boxed{\int_0^1 f(x)\,dx \approx -\frac{1}{6}f(0) + \frac{8}{9}f(0.25) + \frac{5}{18}f(1)}$$

(b) Use the quadrature formula from part (b) to approximate the value of the integral

$$\int_0^1 \frac{1}{1+x^2}\,dx.$$

Solution:

$$\int_0^1 \frac{1}{1+x^2}\,dx \approx -\frac{1}{6}\frac{1}{(1+0^2)} + \frac{8}{9}\frac{1}{(1+0.25^2)} + \frac{5}{18}\frac{1}{(1+1^2)} = 0.808823$$

The exact value is

$$\int_0^1 \frac{1}{1+x^2}\,dx = [\arctan(1) - \arctan(0)] = \frac{\pi}{4}$$

So the absolute error is

$$\boxed{|\pi/4 - 0.0808823| = 0.023425.}$$

Compute the exact value of this integral and find the absolute error of the approximation from part (a).

(c) Show that Gaussian quadrature with 3 nodes and weights

$$\int_{-1}^1 f(x)\,dx \approx \frac{5}{9}f\left(-\sqrt{3/5}\right) + \frac{8}{9}f(0) + \frac{5}{9}f\left(\sqrt{3/5}\right)$$

has degree of precision equal to 5.

Solution:

We need to verify the maximum degree of monomial such that Gaussian quadrature with 3 nodes is exact.

$$\int_{-1}^1 1\,dx = 2 = \frac{5}{9} + \frac{8}{9} + \frac{5}{9} = \frac{18}{9}. \quad \checkmark$$

$$\int_{-1}^1 x\,dx = 0 = -\frac{5}{9}\sqrt{\frac{3}{5}} + \frac{5}{9}\sqrt{\frac{3}{5}}. \quad \checkmark$$

$$\int_{-1}^1 x^2\,dx = \frac{2}{3} = \frac{5}{9}\cdot\frac{3}{5} + \frac{5}{9}\cdot\frac{3}{5}. \quad \checkmark$$

$$\int_{-1}^{1} x^3\,dx = 0 = -\frac{5}{9}\left(\frac{3}{5}\right)^{3/2} + \frac{5}{9}\left(\frac{3}{5}\right)^{3/2}. \quad \checkmark$$

$$\int_{-1}^{1} x^4\,dx = \frac{2}{5} = \frac{5}{9}\left(\frac{9}{25}\right) + \frac{5}{9}\left(\frac{9}{25}\right). \quad \checkmark$$

$$\int_{-1}^{1} x^5\,dx = 0 = -\frac{5}{9}\left(\frac{3}{5}\right)^{5/2} + \frac{5}{9}\left(\frac{3}{5}\right)^{5/2}. \quad \checkmark$$

$$\int_{-1}^{1} x^6\,dx = \frac{2}{7} = \frac{5}{9}\left(\frac{27}{125}\right) + \frac{5}{9}\left(\frac{27}{125}\right) = \frac{6}{25} \quad \text{X}$$

So the degree of precision is equal to 5.

3. (10 points)

(a) The left end-point rule is defined as follows: for nodes x_0 and x_1, approximate the integral by the area of a rectangle whose height is evaluated at the left end-point of the interval. Using Taylor series centered at $x = x_0$, and expanding $f(x)$ up to the linear term only, show that the left end-point rule with remainder is given by

$$\int_{x_0}^{x_1} f(x)\,dx = hf(x_0) + \frac{h^2}{2}f'(c)$$

for some $c \in (x_0, x_1)$.

Solution:

Expand $f(x)$ around $x = x_0$ by Taylor series.

$$f(x) = f(x_0) + (x - x_0)f'(c)$$

for some $c \in (x_0, x_1)$. Integrating both side of the Taylor series on an interval $[x_0, x_1]$

$$\int_{x_0}^{x_1} f(x)\,dx = \int_{x_0}^{x_1} f(x_0)\,dx + \int_{x_0}^{x_1} (x - x_0)f'(c)\,dx$$

Set $h = x_1 - x_0$ and change variables $u = x - x_0$. When $x = x_0$, $u = 0$ and when $x = x_1$, then $u = h$. Then the integral becomes

$$\int_{x_0}^{x_1} f(x)\,dx = f(x_0)\int_0^h du + f'(c)\int_0^h u\,du = \boxed{hf(x_0) + \frac{h^2}{2}f'(c)}$$

(b) Generalize the method developed in part (a) to show that the composite left-end point method with n sub-divisions is given by

$$\int_a^b f(x)\,dx = h\sum_{k=0}^{n-1} f(a + kh) + (b - a)\frac{h}{2}f'(c)$$

where $c \in (a, b)$.

Solution:
Set $h = (b-a)/n$, $a = x_0$, $x_k = a + kh$ and $b = x_n$. Using the left end-points as heights, we have

$$\int_a^b f(x)\,dx = h\left[f(x_0) + f(x_1) + \cdots + f(x_{n-1})\right] + \frac{h^2}{2}\left[f'(c_1) + \cdots + f'(c_n)\right]$$

where there is a c_k for each interval. Using summation notation this is equivalent to

$$\int_a^b f(x)\,dx = h\sum_{k=0}^{n-1} f(x_k) + \frac{h^2}{2}\sum_{k=1}^{n} f'(c_k)$$

The first sum can be rewritten as

$$h\sum_{k=0}^{n-1} f(a+kh).$$

By using the Generalized Intermediate Value Theorem, there exists a c such that second sum is

$$\frac{h^2}{2}\sum_{k=1}^{n} f'(c_k) = \frac{h^2}{2} n f'(c).$$

Since $n = (b-a)/h$ we have

$$\frac{h^2}{2} n f'(c_k) = \frac{h^2}{2}\cdot\frac{(b-a)}{h} f'(c_k).$$

Hence,

$$\boxed{\int_a^b f(x)\,dx = h\sum_{k=0}^{n-1} f(a+kh) + (b-a)\frac{h}{2} f'(c)}$$

as required.

(c) Find the minimum number of sub-divisions n such that the integral

$$\int_0^1 x^2\,dx$$

can be approximated by the left end-point rule up to an error of at most 0.001. Hence find the minimum value of h that corresponds to this n.

Solution:
We want to find n such that the error term is less than 0.001, that is find n such that

$$(b-a)\frac{h}{2} f'(c) \le 0.001$$

We have $f'(c) = 2$, and $b - a = 1$. So

$$\frac{h}{2}\cdot 2 \le 0.001$$

so that $\boxed{h \le 0.001}$ and $n = 1/h = 1/0.001 = \boxed{1,000}$

4. (10 points)

Consider the integral

$$I = \int_0^{\pi} \exp(\sin(x))\, dx \approx 6.208758035711110.$$

(a) Use the Trapezoidal rule with $n = 4$ sub-divisions to approximate I.

Solution:

$$I \approx \frac{h}{2}\left[f(0) + 2f(\pi/4) + 2f(\pi/2) + 2f(3\pi/4) + f(\pi)\right]$$

$$I \approx \frac{\pi}{8}\left[e^{\sin(0)} + 2e^{\sin(\pi/4)} + 2e^{\sin(\pi/2)} + 2e^{\sin(3\pi/4)} + e^{\sin(\pi)}\right] = 6.106087$$

(b) Use Simpson's method with $n = 2 \cdot 2 = 4$ sub-divisions to approximate I.

Solution:

$$I \approx \frac{h}{3}\left[f(0) + f(\pi) + 4f(\pi/4) + 2f(\pi/2) + 4f(3\pi/4)\right]$$

$$I \approx \frac{\pi}{12}\left[e^{\sin(0)} + e^{\sin(\pi)} + 4e^{\sin(\pi/4)} + 2e^{\sin(\pi/2)} + 4e^{\sin(3\pi/4)}\right] = 6.19456$$

(c) Use Gaussian quadrature with $n = 3$ nodes to approximate I.

Solution:

In order to apply Gaussian quadrature on a general interval, we need to tranform the integral as follows

$$\int_a^b f(x)\, dx = \int_{-1}^1 f\left(\frac{(b-a)t + a + b}{2}\right)\frac{b-a}{2}\, dt = \int_{-1}^1 f\left(\pi(t+1)/2\right)\frac{\pi}{2}\, dt$$

where we used $a = 0, b = \pi$. Hence,

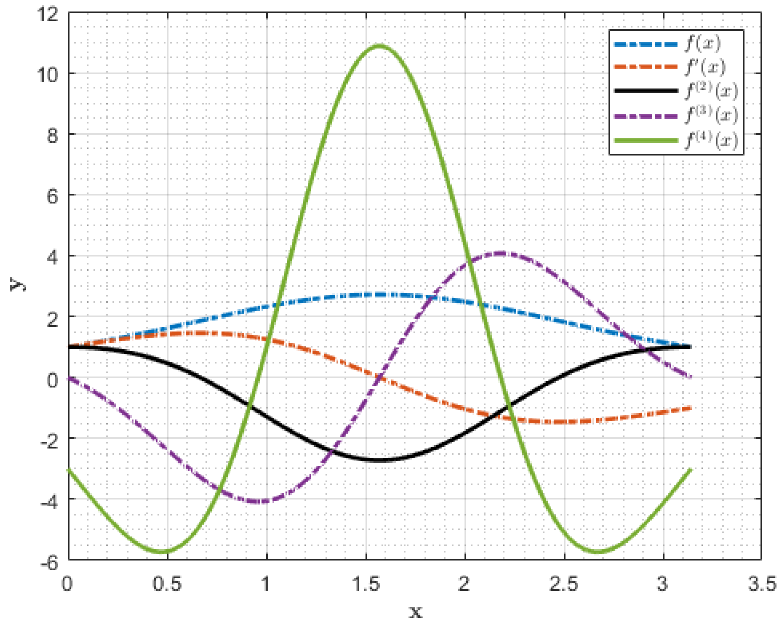
$$\int_0^{\pi} e^{\sin(x)}\, dx \approx \frac{\pi}{2}\left[\frac{5}{9}f\left(\frac{\pi}{2}\left[-\sqrt{3/5}+1\right]\right) + \frac{8}{9}f\left(\frac{\pi}{2}\right) + \frac{5}{9}f\left(\frac{\pi}{2}\left[\sqrt{3/5}+1\right]\right)\right]$$

$$\int_0^{\pi} e^{\sin(x)}\, dx \approx \frac{\pi}{2}\left[\frac{5}{9}e^{\sin\frac{\pi}{2}\left(-\sqrt{3/5}+1\right)} + \frac{8}{9}e^{\sin\left(\frac{\pi}{2}\right)} + \frac{5}{9}e^{\sin\frac{\pi}{2}\left(\sqrt{3/5}+1\right)}\right] = 6.264046$$

(d) The graph of $f(x) = \exp(\sin(x))$ and its derivatives $f'(x)$, $f^{(2)}(x)$, $f^{(3)}(x)$ and $f^{(4)}(x)$ on $[0, \pi]$ is depicted below.

Using information from this graph answer the following questions.

(i) Find the maximum value of h such that Simpson's rule applied to the integral I results in an error not greater than 10^{-3}.



Solution:
The error term for Simpson's rule is

$$-\frac{(b-a)h^4}{180}|f^{(4)}(\xi)|$$

for some $\xi \in (a,b)$. We want to find h such that

$$\frac{(b-a)h^4}{180}|f^{(4)}(\xi)| \leq 10^{-3}.$$

Solving for h, and setting $b-a=\pi$ we have

$$h \leq \left(\frac{180 \cdot 10^{-3}}{\pi|f^{(4)}(\xi)|}\right)^{1/4} = \left(\frac{0.18}{\pi|f^{(4)}(\xi)|}\right)^{1/4}.$$

We need to find **the largest** value of $|f^{(4)}(\xi)|$. From the graph, we see $|f^{(4)}(\xi)| \approx 11$. Hence

$$h \leq \left(\frac{0.18}{11\pi}\right)^{1/4} = 0.2686$$

(ii) Find the number of sub-divisions n such that the Trapezoidal rule applied to I results in an error not greater than 10^{-3}.
Solution:
The error for the Trapezoidal rule is given by

$$\frac{-(b-a)h^2}{12}f^{(2)}(\xi)$$

for some $\xi \in (a, b)$. First let's determine h such that

$$\frac{(b-a)h^2}{12}|f^{(2)}(\xi)| \leq 10^{-3}.$$

Solving for h,

$$h \leq \sqrt{\frac{0.012}{\pi|f^{(2)}(\xi)|}}.$$

To determine the smallest possible right hand side, we need to find the **largest possible** value of $|f^{(2)}(\xi)|$ on the interval $(0, \pi)$. From the graph, this value is around 3. Hence

$$h \leq \sqrt{\frac{0.012}{3\pi}} = 0.0357.$$

The corresponding number of subintervals is then

$$n = (b-a)/h = \pi/0.0357 \approx 88.$$

5. (10 points)

Consider the initial value problem

$$y'(t) = y(t) - e^{-t}, \quad y(0) = 1, \quad t \in [0, 0.01]$$

The exact solution is $y(t) = \frac{1}{2}\left(e^t + e^{-t}\right)$.

(a) Use Euler's method with step size $h = 0.01$ to approximate $y(0.01)$. Compute the absolute error of the approximation at $t = 0.01$.

Solution:

Euler's method is given by the iteration

$$y_{n+1} = y_n + hf(t_n, y_n)$$

. The starting point is $y_0 = 1$ and $f(t, y) = y - e^{-t}$ So

$$y_{n+1} = y_n + h\left[y_n - e^{-t_n}\right].$$

$$y_1 = 1 + 0.01\left[1 - e^{-0}\right] = 1.$$

The absolute error at $t = 0.01$ is

$$|y(0.01) - y_1| = |0.5(e^{0.01} + e^{-0.01}) - 1| = 0.00005 = 5 \times 10^{-5}.$$

(b) The modified Euler's method (Heun's method) is defined as

$$y_{n+1} = y_n + \frac{h}{2}\left[f(t_n, y_n) + f(t_{n+1}, y_n + hf(t_n, y_n))\right], \quad y_0 = y(0).$$

Use the modified Euler's method to approximate the value of $y(0.01)$ using a step size of $h = 0.01$. Compute the absolute error at $t = 0.01$.

Solution:

The iteration for modified Euler in this case is given by

$$y_{n+1} = y_n + \frac{h}{2}\left[y_n - e^{-t_n} + y_n + h(y_n - e^{-t_n}) - e^{-t_{n+1}}\right].$$

Solving for y_{n+1}:

$$y_{n+1} = y_n(1 + h + h^2/2) - e^{-t_n}(h/2 + h^2/2) - \frac{h}{2}e^{-t_{n+1}} = 1.0000497508$$

The absolute error is therefore,

$$|y(0.01) - y_1| = 2.496 \times 10^{-7}.$$

(c) Is the modified Euler's method an explicit or implicit method? Explain.

Solution:

The modified Euler method is an explicit method because the value at the **next** time step y_{n+1} depends only on the value of the solution at the **current** time level y_n.

6. (10 points)

The Crank-Nicholson's scheme for approximating the initial value problem

$$y'(t) = f(t, y(t)), \quad y(0) = y_0$$

is defined as follows

$$y_{n+1} = y_n + \frac{h}{2}\left[f(t_n, y_n) + f(t_{n+1}, y_{n+1})\right]$$

where y_{n+1} is the unknown.

(a) By integrating the ODE on the interval $[t_n, t_{n+1}]$, and using the Trapezoidal rule to approximate the integral, derive the Crank-Nicholson scheme.

Solution:

Integrating the ODE

$$y'(t) = f(t, y)$$

on an interval $[t_n, t_{n+1}]$, we get

$$\int_{t_n}^{t_{n+1}} y'(t)\, dt = \int_{t_n}^{t_{n+1}} f(t, y(t))\, dt$$

By the Fundamental Theorem of Calculus, the left hand integral is evaluated as

$$\int_{t_n}^{t_{n+1}} y'(t)\, dt = y(t_{n+1}) - y(t_n)$$

The right hand side can be approximated by the Trapezoidal rule,

$$\int_{t_n}^{t_{n+1}} f(t, y(t))\, dt = \frac{t_{n+1} - t_n}{2} \left[f(t_n, y(t_n)) + f(t_{n+1}, y(t_{n+1}))\right]$$

Let $h := t_{n+1} - t_n$ and $y_n \approx y(t_n)$. Then we obtain the Crank-Nicholson scheme:

$$\boxed{y_{n+1} = y_n + \frac{h}{2}\left[f(t_n, y_n) + f(t_{n+1}, y_{n+1})\right]}$$

(b) Use the Crank-Nicholson scheme with $h = 0.01$ to approximate $y(0.01)$ for the initial value problem in 5(a). Compute the absolute error at $t = 0.01$

Solution:

The iteration for the Crank-Nicholson scheme in this case is given by

$$y_{n+1} = y_n + \frac{h}{2}\left[y_n - e^{-t_n} + y_{n+1} - e^{-t_{n+1}}\right].$$

Solving for y_{n+1}:

$$y_{n+1}(1 - h/2) = y_n(1 + h/2) - \frac{h}{2}\left(e^{-t_n} + e^{-t_{n+1}}\right)$$

Hence,

$$y_{n+1} = \frac{y_n(1 + h/2) - \frac{h}{2}\left(e^{-t_n} + e^{-t_{n+1}}\right)}{1 - h/2} = \frac{1(1 + 0.005) - 0.005(e^0 + e^{-0.01})}{1 - 0.005}$$

So

$$y_1 = 1.000050000835431.$$

The absolute error is

$$|y(0.01) - y_1| = 4.188 \times 10^{-10}.$$

(c) Is the Crank-Nicholson scheme an explicit or implicit method? Explain.

Solution:

The Crank-Nicholson scheme is an implicit scheme because the solution at the next time step depends on the solution at both the current and the next time step.

(d) Use the fourth-order Runge-Kutta (RK-4) method to approximate $y(0.01)$ for the initial value problem in 5(a). Compute the absolute error at $t = 0.01$.

Solution:

The RK-4 method is defined by the iteration

$$y_{n+1} = y_n + \frac{h}{6}\left[k_1 + 2k_2 + 2k_3 + k_4\right]$$

where

$$\begin{aligned} k_1 &= f(t_n, y_n) \\ k_2 &= f(t_n + h/2, y_n + hk_1/2) \\ k_3 &= f(t_n + h/2, y_n + hk_2/2) \\ k_4 &= f(t_n + h, y_n + hk_3). \end{aligned}$$

In this case, the values of k_i can be computed explicitly as follows,

$$k_1 = y_0 - e^{-t_0} = 1 - e^0 = 0$$

$$\begin{aligned} k_2 &= (y_0 + hk_1/2) - e^{-(t_0+h/2)} = 1 - e^{-0.005} = 0.0049875 \\ k_3 &= (y_0 + hk_2/2) - e^{-(t_0+h/2)} = (1 + 0.01 \cdot 0.0049875/2) - e^{-0.005} = 0.0050125 \\ k_4 &= (y_0 + hk_3) - e^{-t_0+h} = (1 + 0.01 \cdot 0.0050125) - e^{-0.01} = 0.010000. \end{aligned}$$

Therefore,

$$y_1 = 1 + \frac{0.01}{6}\left[0 + 2 \cdot 0.0049875 + 2 \cdot 0.0050125 + 0.010000\right] = 1.00005.$$

The absolute error is

$$|y(0.01) - y_1| = 4.1667 \times 10^{-10}.$$