Scientific Computing HW 3

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Problem 1. Pf. From the Butcher array,

$$A = \begin{bmatrix} \gamma & 0 \\ 1-\gamma & \gamma \end{bmatrix}, \quad b = \begin{bmatrix} 1-\gamma \\ \gamma \end{bmatrix}, \quad c = \begin{bmatrix} \gamma \\ 1 \end{bmatrix}$$

Check the 1st order accuracy condition.

$$\sum_{l=1}^{2} b_l = (1-\gamma) + \gamma = 1$$

Check the 2nd order accuracy condition.

$$\sum_{l=1}^{2} b_l c_l = (1-\gamma)\gamma + \gamma \cdot 1 = \gamma - \gamma^2 + \gamma = 2\gamma - \gamma^2 = 2 - 2^{1/2} - 1 - 2^{-1} + 2^{1/2} = 1 - 2^{-1} = \frac{1}{2}$$

Thus the method is 2nd order accurate. To show it is A–stable, first find the stability function $R(z)$ and let $|z| \to \infty$.

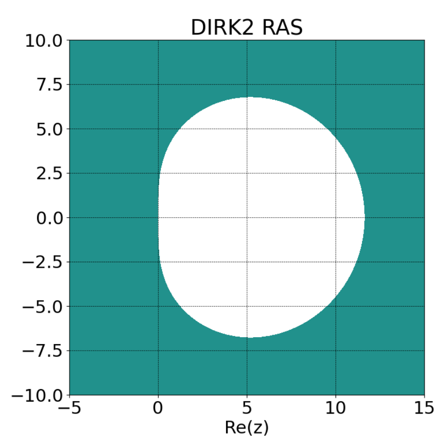
$$I - zA = \begin{bmatrix} 1-\gamma z & 0 \\ -(1-\gamma)z & 1-\gamma z \end{bmatrix} \implies D := \det(I - zA) = (1-\gamma z)^2 = \gamma^2 z^2 - 2\gamma z + 1$$

$$\implies (I - zA)^{-1} = \frac{1}{D} \begin{bmatrix} 1-\gamma z & 0 \\ (1-\gamma)z & 1-\gamma z \end{bmatrix} \implies (I - zA)^{-1} 1_{s\times 1} = \frac{1}{D} \begin{bmatrix} 1-\gamma z \\ (1-\gamma)z + 1 - \gamma z \end{bmatrix} = \frac{1}{D} \begin{bmatrix} 1-\gamma z \\ (1-2\gamma)z + 1 \end{bmatrix}$$

$$R(z) - 1 = zb^T (I - zA)^{-1} 1_{s\times 1} = \frac{z}{D} \left[(1-\gamma)(1-\gamma z) + \gamma((1-2\gamma)z+1)\right] = \frac{z}{D}\left[1 - \gamma z - \gamma + \gamma^2 z + (\gamma - 2\gamma^2)z + \gamma\right]$$

$$\implies R(z) - 1 = \frac{z}{D}\left[1 - \gamma^2 z\right] = \frac{-\gamma^2 z^2 + z}{\gamma^2 z^2 - 2\gamma z + 1} \implies R(z) = \frac{-\gamma^2 z^2 + z}{\gamma^2 z^2 - 2\gamma z + 1} + 1 \xrightarrow{|z|\to\infty} -1 + 1 = 0$$

To finish showing A–stability, we plot the RAS and see that it contains the left half plane. Code in 2nd cell of:
`https://github.com/RokettoJanpu/Scientific-Computing-2/blob/main/hw3%20RAS.ipynb`



Problem 2. From the Butcher array,

$$A = \begin{bmatrix} \gamma & 0 \\ 1-2\gamma & \gamma \end{bmatrix}, b = \begin{bmatrix} 1/2 \\ 1/2 \end{bmatrix}, c = \begin{bmatrix} \gamma \\ 1-\gamma \end{bmatrix}$$

1. **Pf.** Check the 1st order accuracy condition.

$$\sum_{l=1}^{2} b_l = \frac{1}{2} + \frac{1}{2} = 1$$

Check the 2nd order accuracy condition.

$$\sum_{l=1}^{2} b_l c_l = \frac{1}{2}\gamma + \frac{1}{2}(1-\gamma) = \frac{1}{2}(\gamma + 1 - \gamma) = \frac{1}{2}$$

2. **Pf.** Check the 3rd order accuracy conditions.

$$\sum_{p,q,r} b_p a_{pq} a_{pr} = \frac{1}{2}[\gamma^2 + 2\gamma \cdot 0 + 0^2] + \frac{1}{2}[(1-2\gamma)^2 + 2(1-2\gamma)\gamma + \gamma^2]$$

The quantity in the second bracket is

$$(1-2\gamma)^2 + 2(1-2\gamma)\gamma + \gamma^2 = 1 + 4\gamma^2 - 4\gamma + 2\gamma - 4\gamma^2 + \gamma^2 = \gamma^2 - 2\gamma + 1 = (\gamma - 1)^2$$

giving

$$\sum_{p,q,r} b_p a_{pq} a_{pr} = \frac{1}{2}[\gamma^2 + \gamma^2 - 2\gamma + 1] = \gamma^2 - \gamma + \frac{1}{2}$$

We find

$$\gamma^2 = \frac{1}{2} + \frac{3}{36} + 2\frac{3^{1/2}}{12} = \frac{1}{12}[3 + 1 + 2 \cdot 3^{1/2}] = \frac{1}{12}[4 + 2 \cdot 3^{1/2}] = \frac{1}{6}[2 + 3^{1/2}]$$

so finally,

$$\sum_{p,q,r} b_p a_{pq} a_{pr} = \frac{1}{6}[2 + 3^{1/2} - 3 - 3^{1/2} + 3] = \frac{1}{3}$$

3. First find the stability function $R(z)$.

$$I - zA = \begin{bmatrix} 1-\gamma z & 0 \\ -(1-2\gamma)z & 1-\gamma z \end{bmatrix} \implies D := \det(I - zA) = (1-\gamma z)^2 = \gamma^2 z^2 - 2\gamma z + 1$$

$$\implies (I - zA)^{-1} = \frac{1}{D}\begin{bmatrix} 1-\gamma z & 0 \\ (1-2\gamma)z & 1-\gamma z \end{bmatrix} \implies (I-zA)^{-1}1_{s\times 1} = \frac{1}{D}\begin{bmatrix} 1-\gamma z \\ (1-2\gamma)z + 1 - \gamma z \end{bmatrix} = \frac{1}{D}\begin{bmatrix} 1-\gamma z \\ (1-3\gamma)z + 1 \end{bmatrix}$$

$$R(z) - 1 = zb^T(I-zA)^{-1}1_{s\times 1} = \frac{z}{2D}\left[1 - \gamma z + (1-3\gamma)z + 1)\right] = \frac{z}{2D}\left[(1-4\gamma)z + 2\right] = \frac{1}{2}\frac{(1-4\gamma)z^2 + 2z}{\gamma^2 z^2 - 2\gamma z + 1}$$

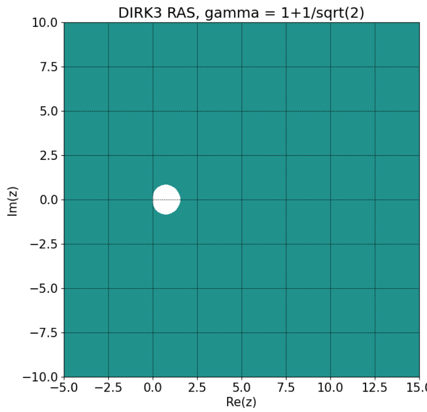
We find γ by imposing $\lim_{|z|\to\infty} R(z) = 0$.

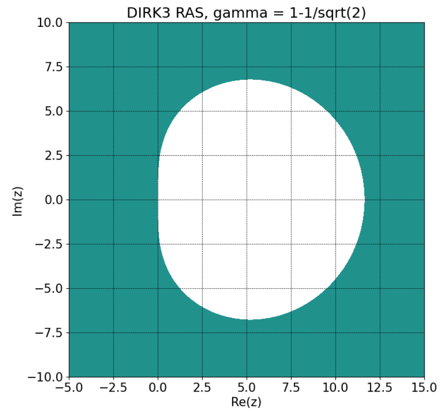
$$\lim_{|z|\to\infty} R(z) = 0 \iff -1 = \frac{1}{2}\lim_{|z|\to\infty}\frac{(1-4\gamma)z^2 + 2z}{\gamma^2 z^2 - 2\gamma z + 1} \iff \lim_{|z|\to\infty}\frac{(1-4\gamma)z^2 + 2z}{\gamma^2 z^2 - 2\gamma z + 1} = -2 \iff \frac{1-4\gamma}{\gamma^2} = -2$$

$$\iff -2\gamma^2 = 1 - 4\gamma \iff 2\gamma^2 - 4\gamma + 1 = 0 \iff \gamma = \frac{4}{4} \pm \frac{(16-8)^{1/2}}{4} = 1 \pm \frac{2 \cdot 2^{1/2}}{4} = 1 \pm 2^{-1/2}$$

We check that the method for $\gamma = 1 \pm 2^{-1/2}$ is A–stable, hence L–stable, by plotting the RASes and seeing that they contain the left half plane. Code in 3rd cell of:

`https://github.com/RokettoJanpu/Scientific-Computing-2/blob/main/hw3%20RAS.ipynb`





Problem 3. Code for all parts of this problem:
`https://github.com/RokettoJanpu/Scientific-Computing-2/blob/main/hw3.ipynb`

(a) Set $f(t,y) := -L(y-\phi(t)) + \phi'(t)$. To implement DIRK2, we first obtain explicit formulas for k_1, k_2, u_{n+1}.

$$k_1 = f(t_n+\gamma h, u_n + h\gamma k_1) = -L\left[u_n + h\gamma k_1 - \phi(t_n+\gamma h)\right] + \phi'(t_n+\gamma h)$$

$$\implies k_1 = -Lh\gamma k_1 - L\left[u_n - \phi(t_n+\gamma h)\right] + \phi'(t_n+\gamma h)$$

$$\implies (1+Lh\gamma)k_1 = -L\left[u_n - \phi(t_n+\gamma h)\right] + \phi'(t_n+\gamma h) \implies k_1 = \frac{-L\left[u_n - \phi(t_n+\gamma h)\right] + \phi'(t_n+\gamma h)}{1+Lh\gamma}$$

$$k_2 = f(t_n+h, u_n + h(1-\gamma)k_1 + h\gamma k_2) = -L\left[u_n + h(1-\gamma)k_1 + h\gamma k_2 - \phi(t_n+h)\right] + \phi'(t_n+h)$$

$$\implies k_2 = -Lh\gamma k_2 - L\left[u_n + h(1-\gamma)k_1 - \phi(t_n+h)\right] + \phi'(t_n+h)$$

$$\implies (1+Lh\gamma)k_2 = -L\left[u_n + h(1-\gamma)k_1 - \phi(t_n+h)\right] + \phi'(t_n+h)$$

$$\implies k_2 = \frac{-L\left[u_n + h(1-\gamma)k_1 - \phi(t_n+h)\right] + \phi'(t_n+h)}{1+Lh\gamma}$$

$$u_{n+1} = u_n + h\left[(1-\gamma)k_1 + \gamma k_2\right]$$

We do the same for DIRK3 (abuse of notation for DIRK of order 3).

$$k_1 = f(t_n+\gamma h, u_n + h\gamma k_1)$$

so the explicit formula for k_1 is the same as in DIRK2.

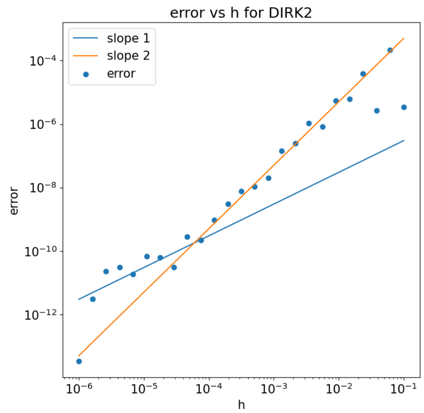
$$k_1 = \frac{-L\left[u_n - \phi(t_n+\gamma h)\right] + \phi'(t_n+\gamma h)}{1+Lh\gamma}$$

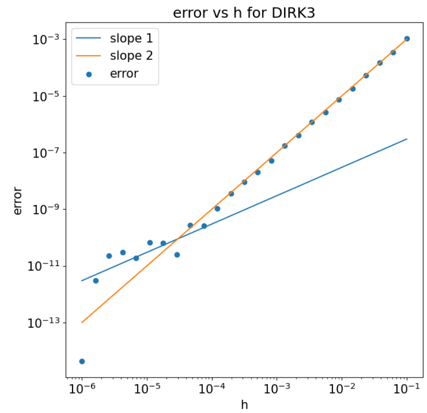
$$\begin{aligned} k_2 &= f(t_n+(1-\gamma)h, u_n + h(1-2\gamma)k_2 + h\gamma k_2) \\ &= -L\left[u_n + h(1-2\gamma)k_1 + h\gamma k_2 - \phi(t_n+(1-\gamma)h)\right] + \phi'(t_n+(1-\gamma)h) \\ &= -Lh\gamma k_2 - L\left[u_n + h(1-2\gamma)k_1 - \phi(t_n+(1-\gamma)h)\right] + \phi'(t_n+(1-\gamma)h) \end{aligned}$$

$$\implies (1+Lh\gamma)k_2 = -L\left[u_n + h(1-2\gamma)k_1 - \phi(t_n+(1-\gamma)h)\right] + \phi'(t_n+(1-\gamma)h)$$

$$\implies k_2 = \frac{-L\left[u_n + h(1-2\gamma)k_1 - \phi(t_n+(1-\gamma)h)\right] + \phi'(t_n+(1-\gamma)h)}{1+Lh\gamma}$$

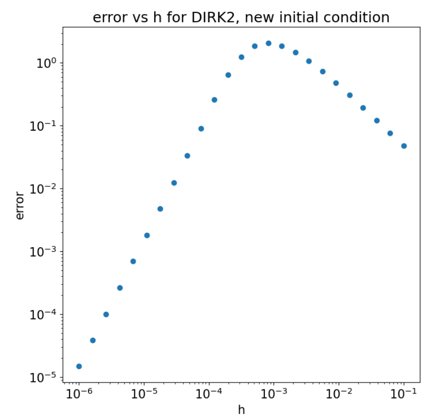
$$u_{n+1} = u_n + \frac{h}{2}[k_1 + k_2]$$

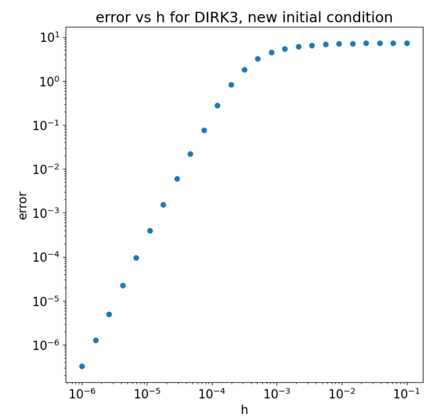




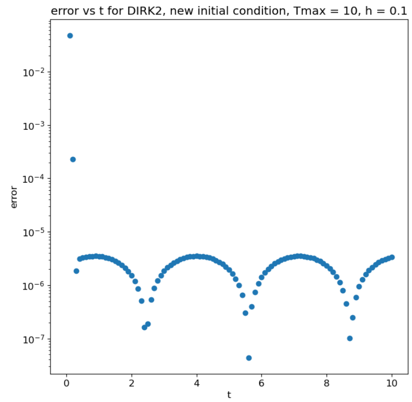
For $h > 10^{-4}$, the log–log graph roughly has a slope of 2, ie the error is on the order of h. For $10^{-5} < h < 10^{-4}$, the log–log graph roughly has a slope of 1, ie the error is on the order of h^2. For $h < 10^{-5}$, the slope is considerably steeper, ie the error is on the order of a high power of h.

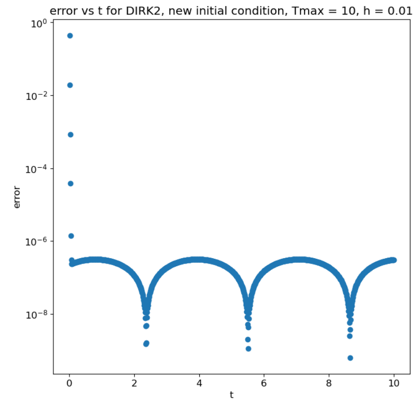
(b) Repeating (a) with $y(0) = \sin\left(\frac{\pi}{4}\right) + 10$, we notably get a region for DIRK2 where error increases as h decreases, and a region for DIRK3 of very small slope.

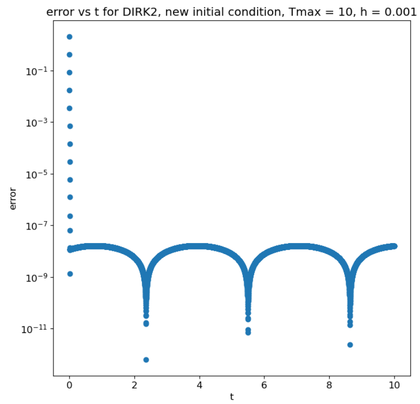


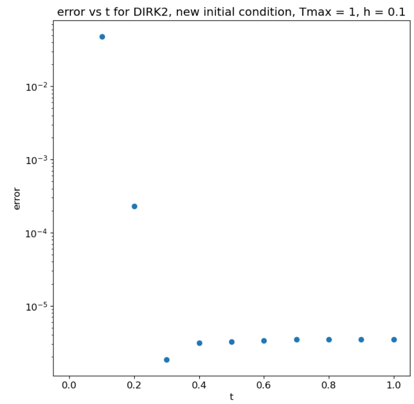


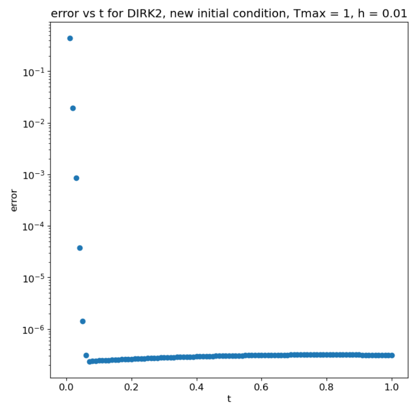
For each method, we plot error vs time graphs for $h = 10^{-1}, 10^{-2}, 10^{-3}$ and $T_{\max} = 10, 1$.

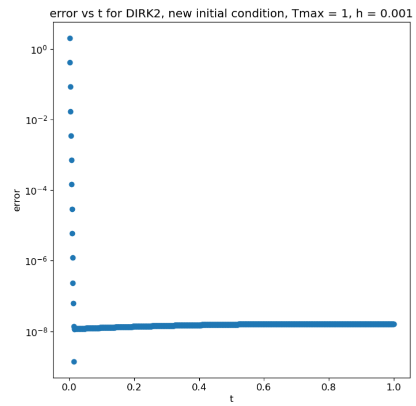

error vs t for DIRK2, new initial condition, Tmax = 10, h = 0.1
error
t

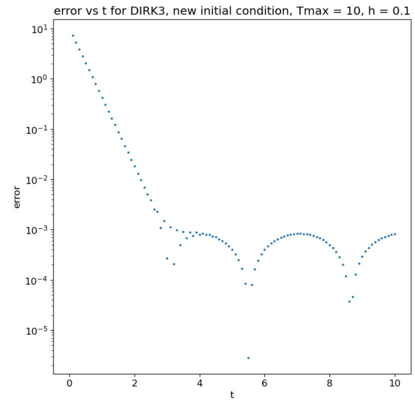

error vs t for DIRK2, new initial condition, Tmax = 10, h = 0.01
error
t

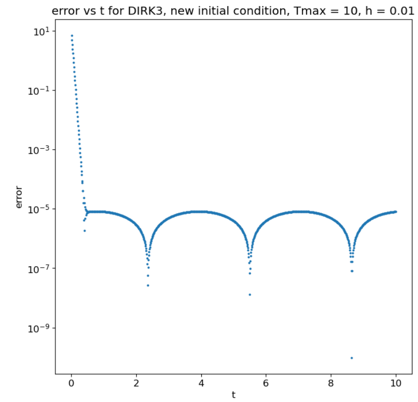

error vs t for DIRK2, new initial condition, Tmax = 10, h = 0.001
error
t

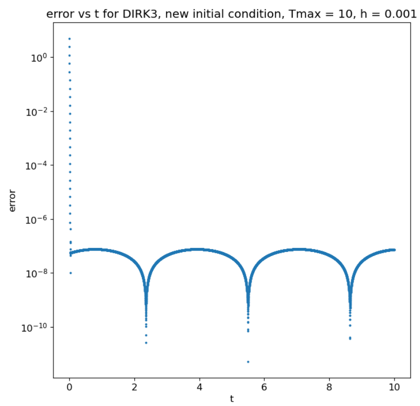

error vs t for DIRK2, new initial condition, Tmax = 1, h = 0.1
error
t

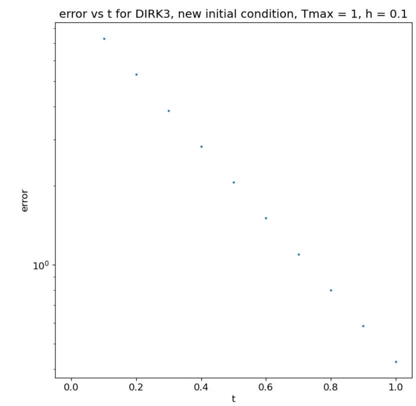

error vs t for DIRK2, new initial condition, Tmax = 1, h = 0.01
error
t

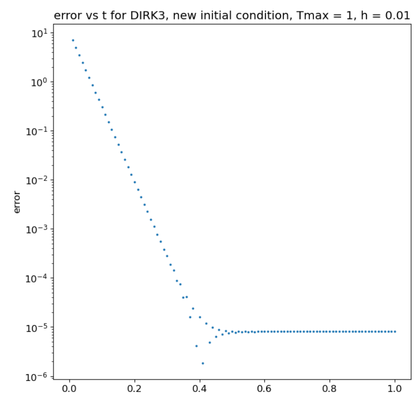

error vs t for DIRK2, new initial condition, Tmax = 1, h = 0.001
error
t

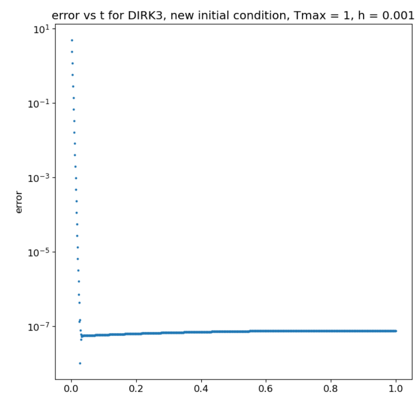












(c) When the initial condition receives a

Problem 3. For the three–step Adams–Moulton method, Newton's interpolant is

$$p(t) = f_{n+1} + f[t_{n+1}, t_n](t - t_{n+1}) + f[t_{n+1}, t_n, t_{n-1}](t - t_{n+1})(t - t_n) + f[t_{n+1}, t_n, t_{n-1}, t_{n-2}](t - t_{n+1})(t - t_n)(t - t_{n-1})$$

Define

$$a(t) = f_{n+1}, b(t) = f[t_{n+1}, t_n](t - t_{n+1}), c(t) = (t - t_{n+1})(t - t_n), d(t) = (t - t_{n+1})(t - t_n)(t - t_{n=1})$$

The method is

$$u_{n+1} = u_n + \int_{t_n}^{t_{n+1}} p(t)dt = u_n + \int_{t_n}^{t_{n+1}} a(t)dt + \int_{t_n}^{t_{n+1}} b(t)dt$$
$$+ f[t_{n+1}, t_n, t_{n-1}] \int_{t_n}^{t_{n+1}} c(t)dt + f[t_{n+1}, t_n, t_{n-1}, t_{n-2}] \int_{t_n}^{t_{n+1}} d(t)dt \quad (3.1)$$

Define a variable timestep $h_n := t_{n+1} - t_n$. The first two integrals are found by

$$\int_{t_n}^{t_{n+1}} a(t)dt = f_{n+1}t \Big|_{t_n}^{t_{n+1}} = f_{n+1}(t_{n+1} - t_n) = f_{n+1}h_n$$

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

We do some algebra before finding the third integral.

$$c(t) = (t - t_{n+1})(t - t_n) = t^2 - (t_n + t_{n+1})t + t_{n+1}t_n$$

$$\int_{t_n}^{t_{n+1}} c(t)dt = \frac{1}{3}t^3 - \frac{1}{2}(t_n + t_{n+1})t^2 + t_{n+1}t_n t \Big|_{t_n}^{t_{n+1}} = \frac{1}{3}(t_{n+1}^3 - t_n^3) - \frac{1}{2}(t_n + t_{n+1})(t_{n+1}^2 - t_n^2) + t_{n+1}t_n(t_{n+1} - t_n)$$
$$= \frac{1}{3}(t_{n+1} - t_n)(t_{n+1}^2 + t_{n+1}t_n + t_n^2) - \frac{1}{2}(t_{n+1} - t_n)(t_{n+1} + t_n)^2 + t_{n+1}t_n h_n$$
$$= h_n \left[\frac{1}{3}(t_{n+1}^2 + t_{n+1}t_n + t_n^2) - \frac{1}{2}(t_{n+1}^2 + t_n^2 + 2t_{n+1}t_n) + t_{n+1}t_n\right] = h_n \left[-\frac{1}{6}t_{n+1}^2 - \frac{1}{6}t_n^2 + \frac{1}{3}t_{n+t}t_n\right]$$
$$= -\frac{1}{6}h_n[t_{n+1}^2 + t_n^2 - 2t_{n+1}t_n] = -\frac{1}{6}h_n[t_{n+1} - t_n]^2 = -\frac{1}{6}h_n^3$$

We handle the fourth integral similarly.

$$d(t) = (t - t_{n+1})(t - t_n)(t - t_{n-1}) = [t^2 - (t_n + t_{n+1})t + t_{n+1}t_n](t - t_{n-1})$$
$$= t^3 - t_{n-1}t^2 - (t_n + t_{n+1})t^2 + (t_n + t_{n+1})t_{n-1}t + t_{n+1}t_n t - t_{n+1}t_n t_{n-1}$$
$$= t^3 - (t_{n+1} + t_n + t_{n-1})t^2 + (t_n t_{n-1} + t_{n+1}t_{n-1} + t_{n+1}t_n)t - t_{n+1}t_n t_{n-1}$$

$$\int_{t_n}^{t_{n+1}} d(t)dt = \frac{1}{4}t^4 - \frac{1}{3}(t_{n+1} + t_n + t_{n-1})t^3 + \frac{1}{2}(t_n t_{n-1} + t_{n+1}t_{n-1} + t_{n+1}t_n)t^2 - t_{n+1}t_n t_{n-1}t \Big|_{t_n}^{t_{n+1}}$$
$$= \frac{1}{4}(t_{n+1}^4 - t_n^4) - \frac{1}{3}(t_{n+1} + t_n + t_{n-1})(t_{n+1}^3 - t_n^3) + \frac{1}{2}(t_n t_{n-1} + t_{n+1}t_{n-1} + t_{n+1}t_n)(t_{n+1}^2 - t_n^2) - t_{n+1}t_n t_{n-1}(t_{n+1} - t_n)$$

$$= \frac{1}{4}(t_{n+1}^2 + t_n^2)(t_{n+1} + t_n)h_n - \frac{1}{3}(t_{n+1} + t_n + t_{n-1})(t_{n+1}^2 + t_{n+1}t_n + t_n^2)h_n$$
$$+ \frac{1}{2}(t_n t_{n-1} + t_{n+1}t_{n-1} + t_{n+1}t_n)(t_{n+1} + t_n)h_n - t_{n+1}t_n t_{n-1}h_n$$
$$= h_n \Bigg[\frac{1}{4}(t_{n+1}^3 + t_{n+1}^2 t_n + t_n^2 t_{n+1}t_n^3) - \frac{1}{3}(t_{n+1}^3 + t_{n+1}^2 t_n + t_{n+1}t_n^2 + t_n t_{n+1}^2 + t_{n+1}t_n^2 + t_n^3 + t_{n-1}t_{n+1}^2 + t_{n+1}t_n t_{n-1} + t_{n-1}t_n^2)$$
$$+ \frac{1}{2}(t_n t_{n-1}t_{n+1} + t_n^2 t_{n-1} + t_{n+1}^2 t_{n-1} + t_{n+1}t_{n-1}t_n + t_{n+1}^2 t_n + t_{n+1}t_n^2) - t_{n+1}t_n t_{n-1}\Bigg]$$