5.11 Determine the characteristic polynomials $\rho(\zeta)$ and $\sigma(\zeta)$ for the following linear multistep methods. Verify that (5.48) holds in each case.
a. The 3-step Adams-Bashforth method.
b. The 3-step Adams-Moulton method.
c. The 2-step Simpson's method of Example 5.16.

Solution.
a. We have that the 3-step Adams-Bashforth method is given by

$$U^{n+3} = U^{n+2} + \frac{h}{12}(5f(U^n) - 16f(U^{n+1}) + 23f(U^{n+2}))$$

Hence

$$U^{n+3} - U^{n+2} = \frac{h}{12}(5f(U^n) - 16f(U^{n+1}) + 23f(U^{n+2}))$$

So, the characteristic polynomials are given by

$$\rho(\zeta) = \zeta^3 - \zeta^2$$
$$\sigma(\zeta) = \frac{23}{12}\zeta^2 - \frac{4}{3}\zeta + \frac{5}{12}$$

Now, we see that

$$\sum_{j=0}^{r} \alpha_j = 1 + (-1) + 0 + 0 = 0$$
$$\sum_{j=0}^{r} \beta_j = \frac{23}{12} - \frac{4}{3} + \frac{5}{12} = 1 = 3(1) + 2(-1) = \sum_{j=0}^{r} j\alpha_j$$

Thus, condition (5.48) holds.

b. We have that the 3-step Adams-Moulton method is given by

$$U^{n+3} = U^{n+2} + \frac{h}{24}(f(U^n) - 5f(U^{n+1}) + 19f(U^{n+2}) + 9f(U^{n+3}))$$

Hence

$$U^{n+3} - U^{n+2} = \frac{h}{24}(f(U^n) - 5f(U^{n+1}) + 19f(U^{n+2}) + 9f(U^{n+3}))$$

So, the characteristic polynomials are given by

$$\rho(\zeta) = \zeta^3 - \zeta^2$$
$$\sigma(\zeta) = \frac{3}{8}\zeta^3 + \frac{19}{24}\zeta^2 - \frac{5}{24}\zeta + \frac{1}{24}$$

Now, we see that

$$\sum_{j=0}^{r} \alpha_j = 1 + (-1) + 0 + 0 = 0$$
$$\sum_{j=0}^{r} \beta_j = \frac{3}{8} + \frac{19}{24} - \frac{5}{24} + \frac{1}{24} = 1 = 3(1) + 2(-1) = \sum_{j=0}^{r} j\alpha_j$$

Thus, condition (5.48) holds.

c. We have that the 2-step Simpson's method is given by

$$U^{n+2} = U^n + \frac{2h}{6}(f(U^n) + 4f(U^{n+1}) + f(U^{n+2}))$$

Hence

$$U^{n+2} - U^n = \frac{2h}{6}(f(U^n) + 4f(U^{n+1}) + f(U^{n+2}))$$

So, the characteristic polynomials are given by

$$\rho(\zeta) = \zeta^2 - 1, \;\; \sigma(\zeta) = \frac{1}{3}\zeta^2 + \frac{4}{3}\zeta + \frac{1}{3}$$

Now, we see that

$$\sum_{j=0}^{r} \alpha_j = 1 + 0 - 1 = 0$$
$$\sum_{j=0}^{r} \beta_j = \frac{1}{3} + \frac{4}{3} + \frac{1}{3} = 2 = 2(1) + 0(-1) = \sum_{j=0}^{r} j\alpha_j$$

Thus, condition (5.48) holds.

5.12 a. Verify that the predictor-corrector method (5.53) is second order accurate.
b. Show that the predictor-corrector method obtained by predicting with the 2-step Adams-Bashforth method followed by correcting with the 2-step Adams-Moulton method is third order accurate.

Solution.
a. We have that the predictor-corrector mathod is given by

$$\hat{U}^{n+1} = U^n + kf(U^n)$$

$$U^{n+1} = U^n + \frac{1}{2}k(f(U^n) + f(\hat{(U)}^{n+1}))$$

So, employing substitution, we get

$$U^{n+1} = U^n + \frac{1}{2}k(f(U^n) + f(U^n + kf(U^n)))$$

Hence,

$$\frac{2(U^{n+1} - U^n)}{k} = f(U^n) + f(U^n + kf(U^n))$$

This gives us the local truncation error

$$\tau = \frac{2}{k}u_{n+1} - \frac{2}{k}u_n - f(u_n) - f(u_n + kf(u_n))$$

Using $u' = \lambda u = f(u)$, we see that

$$\tau = \frac{2}{k}u_{n+1} - \frac{2}{k}u_n - \lambda u_n - \lambda(u_n + k\lambda u_n)$$

Now, expanding u_{n+1} about u_n using Taylor series yields

$$\begin{aligned}\tau = \frac{2}{k}(u_n + ku_n' + \frac{k^2}{2}u_n'' + \mathcal{O}(k^3) - u_n) - \lambda u_n - \lambda(u_n + k\lambda u_n)\\ = 2u_n' + ku_n'' + \mathcal{O}(k^2) - \lambda u_n - \lambda(u_n + k\lambda u_n)\\ = 2\lambda u_n + k\lambda^2 u_n + \mathcal{O}(k^2) - \lambda u_n - \lambda u_n - k\lambda^2 u_n = \mathcal{O}(k^2)\end{aligned}$$

since $u' = \lambda u$. Therefore, the predictor-corrector method is second order accurate as desired.

b. We have that the 2-step AB method is $U^{n+2} = U^{n+1} + \frac{k}{2}(-f(U^n) + 3f(U^{n+1}))$ and the 2-step AM method is $U^{n+2} = U^{n+1} + \frac{k}{12}(-f(U^n) + 8f(U^{n+1}) + 5f(U^{n+2}))$. So,

$$U^{n+2} = U^{n+1} + \frac{k}{12}(-f(U^n) + 8f(U^{n+1}) + 5f(U^{n+1} + \frac{k}{2}(-f(U^n) + 3f(U^{n+1}))))$$

Hence,

$$\frac{12(U^{n+2} - U^{n+1})}{k} = -f(U^n) + 8f(U^{n+1}) + 5f(U^{n+1} + \frac{k}{2}(-f(U^n) + 3f(U^{n+1})))$$

Whence,

$$\frac{12(U^{n+2} - U^{n+1})}{k} + f(U^n) - 8f(U^{n+1}) - 5f(U^{n+1} + \frac{k}{2}(-f(U^n) + 3f(U^{n+1}))) = 0$$

Now, let u_n be the exact solution to the approximation U^n. Also, we will use $u' = \lambda u = f(u)$. So, we get that the local truncation error is

$$\begin{aligned}
\tau &= \frac{12(u_{n+2} - u_{n+1})}{k} + f(u_n) - 8f(u_{n+1}) - 5f(u_{n+1} + \frac{k}{2}(-f(u_n) + 3f(u_{n+1}))) \\
&= \frac{12}{k}u_{n+2} - \frac{12}{k}u_{n+1} + \lambda u_n - 8\lambda u_{n+1} - 5\lambda(u_{n+1} + \frac{k}{2}(-\lambda u_n + 3\lambda u_{n+1})) \\
&= \frac{12}{k}u_{n+2} - \frac{12}{k}u_{n+1} + \lambda u_n - 8\lambda u_{n+1} - 5\lambda(u_{n+1} - \frac{k}{2}\lambda u_n + \frac{3k}{2}\lambda u_{n+1})
\end{aligned}$$

Now, expanding out all u_{n+2} and u_n terms using Taylor series yields

$$\tau = \frac{12}{k}(u_{n+1} + ku'_{n+1} + \frac{k^2}{2}u''_{n+1} + \frac{k^3}{6}u'''_{n+1} + \mathcal{O}(k^4) - u_{n+1}) + \lambda(u_{n+1} - ku'_{n+1} + \frac{k^2}{2}u''_{n+1} + \mathcal{O}(k^3))$$

$$-8\lambda u_{n+1} - 5\lambda(u_{n+1} - \frac{k}{2}(u_{n+1} - ku'_{n+1} + \mathcal{O}(k^2)) + \frac{3k}{2}\lambda u_{n+1})$$

Finally, using $u' = \lambda u$ again, nets us

$$\tau = 12\lambda u_{n+1} + 6k\lambda u_{n+1} + 2k^2\lambda^3 u_{n+1} + \mathcal{O}(k^3) + \lambda u_{n+1} - k\lambda^2 u_{n+1} + \frac{k^2\lambda^3}{2}u_{n+1} + \mathcal{O}(k^3)$$

$$-8\lambda u_{n+1} - 5\lambda u_{n+1} + \frac{5k\lambda}{2}u_{n+1} - \frac{5k^2\lambda^2}{2}u_{n+1} + \mathcal{O}(k^3) - \frac{15k}{2}\lambda^2 u_{n+1}$$

Therefore, we see that the predictor-corrector method obtained by predicting with the 2-step Adams-Bashforth method followed by correcting with the 2-step Adams-Moulton method is third order accurate as desired.

5.13 Consider the Runge-Kutta methods defined by the tableaux below. In each case show that the method is third order accurate in two different ways: First by checking that the order conditions (5.35), (5.38), and (5.39) are satisfied, and then by applying one step of the method to $u' = \lambda u$ and verifying that the Taylor series expansion of $e^{k\lambda}$ is recovered to the expected order.

a.

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & \frac{1}{6} & \frac{2}{3} & 0 & \frac{1}{6} \end{array}$$

b.

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ \frac{2}{3} & 0 & \frac{2}{3} & 0 \\ \hline & \frac{1}{4} & 0 & \frac{3}{4} \end{array}$$

Solution.

a. We first need that $\sum_{j=1}^{r} a_{ij} = c_i$ and $\sum_{j=1}^{r} b_j = 1$. Clearly, $\sum_{j=1}^{r} b_j = \frac{1}{6} + \frac{2}{3} + \frac{1}{6} = 1$. Also, $\sum_{j=1}^{r} a_{1j} = 0 = c_1$, $\sum_{j=1}^{r} a_{2j} = \frac{1}{2} = c_2$, $\sum_{j=1}^{r} a_{3j} = 1 = c_3$, and $\sum_{j=1}^{r} a_{4j} = 1 = c_4$. Now, we need $\sum_{j=1}^{r} b_j c_j = \frac{1}{2}$. We see that $\sum_{j=1}^{r} b_j c_j = (\frac{1}{6}\cdot 0)+(\frac{2}{3}\cdot\frac{1}{2})+(0\cdot 1)+(\frac{1}{6}\cdot 1) = \frac{1}{2}$. Finally, we need $\sum_{j=1}^{r} b_j c_j^2 = \frac{1}{3}$ and $\sum_{i=1}^{r}\sum_{j=1}^{r} b_i a_{ij} c_j = \frac{1}{6}$. We note that $\sum_{j=1}^{r} b_j c_j^2 = (\frac{1}{6}\cdot 0) + (\frac{2}{3}\cdot\frac{1}{4}) + (0\cdot 1) + (\frac{1}{6}\cdot 1) = \frac{1}{3}$ and that $\sum_{i=1}^{r}\sum_{j=1}^{r} b_i a_{ij} c_j = (0) + (0) + (0 + 0 + (\frac{1}{6}\cdot 1\cdot 1) + 0) + (0) = \frac{1}{6}$. So, we have that the third order Rugne-Kutta method is indeed third order accurate.

Now, we will use one step of this third order method to verify the Taylor series expansion of $e^{k\lambda}$ is third order accurate. So,

$$Y_1 = u_n$$
$$Y_2 = u_n + \frac{k}{2} f(Y_1, t_n) = u_n + \frac{k\lambda}{2} u_n$$
$$Y_3 = u_n + kf(Y_2, t_n + \frac{1}{2}k) = u_n + k\lambda u_n + \frac{1}{2}k^2\lambda^2 u_n$$
$$Y_4 = u_n + kf(Y_3, t_n + k) = u_n + k\lambda u_n + k^2\lambda^2 u_n + \frac{1}{2}k^3\lambda^3 u_n$$

$$U^{n+1} = u_n + k(\frac{1}{6}(\lambda u_n) + \frac{2}{3}(\lambda u_n + k\lambda^2 u_n + \frac{1}{2}k^2\lambda^3 u_n) + \frac{1}{6}(\lambda u_n + k\lambda^2 u_n + k^2\lambda^3 u_n + \frac{1}{2}k^3\lambda^4 u_n))$$

$$= u_n + \frac{1}{6}(k\lambda u_n) + \frac{2}{3}(k\lambda u_n + k^2\lambda^2 u_n + \frac{1}{2}k^3\lambda^3 u_n) + \frac{1}{6}(k\lambda u_n + k^2\lambda^2 u_n + k^3\lambda^3 u_n + \frac{1}{2}k^4\lambda^4 u_n)$$

Thus, we have that $e^{k\lambda}$ is recovered to third order accuracy.

b. We will verify the same conditions as in part a above. First, we see that $\sum_{j=1}^{r} a_{1j} = 0 = c_1, \sum_{j=1}^{r} a_{2j} = \frac{1}{3} = c_2$, and $\sum_{j=1}^{r} a_{3j} = \frac{2}{3} = c_3$ and that $\sum_{j=1}^{r} b_j = \frac{1}{4} + \frac{3}{4} = 1$. So, the first condition holds. Now, note that $\sum_{j=1}^{r} b_j c_j = (\frac{1}{4}\cdot 0)+(0\cdot\frac{1}{3})+(\frac{3}{4}\cdot\frac{2}{3}) = \frac{1}{2}$. Hence, the second condition holds. Finally, observe that $\sum_{j=1}^{r} b_j c_j^2 = (\frac{1}{4}\cdot 0)+(0\cdot\frac{1}{9})+(\frac{3}{4}\cdot\frac{4}{9}) = \frac{1}{3}$ and $sum_{i=1}^{r}\sum_{j=1}^{r} b_i a_{ij} c_j = (0) + (0) + (0 + (\frac{3}{4}\cdot\frac{2}{3}\cdot\frac{1}{3}) + 0) = \frac{1}{6}$. Hence, Heun's third order method is thrid order accurate.
Now, we will use one step of this third order method to verify the Taylor series expansion of $e^{k\lambda}$ is third order accurate. So,

$$
\begin{aligned}
Y_1 &= u_n \\
Y_2 &= u_n + \frac{k}{3} f(Y_1, t_n) = u_n + \frac{k\lambda}{3} u_n \\
Y_3 &= u_n + \frac{2}{3} k f(Y_2, t_n + \frac{1}{3}k) = u_n + \frac{2}{3} k\lambda u_n + \frac{1}{3} k^2 \lambda^2 u_n
\end{aligned}
$$

$$
\begin{aligned}
U^{n+1} &= u_n + k(\frac{1}{4}(\lambda u_n) + \frac{3}{4}(\lambda u_n + \frac{2}{3} k\lambda^2 u_n + \frac{1}{3} k^2 \lambda^3 u_n)) \\
&= u_n + \frac{1}{4}(k\lambda u_n) + \frac{3}{4}(k\lambda u_n + \frac{2}{3} k^2\lambda^2 u_n + \frac{1}{3} k^3 \lambda^3 u_n)
\end{aligned}
$$

Thus, we have that $e^{k\lambda}$ is recovered to third order accuracy.

5.17 a. Apply the trapezoidal method to the equation $u' = \lambda u$ and show that

$$U^{n+1} = (\frac{1 + z/2}{1 - z/2})U^n$$

where $z = k\lambda$.

b. Let

$$R(z) = \frac{1 + z/2}{1 - z/2}$$

Show that $R(z) = e^z + \mathcal{O}(z^3)$ and conclude that the one-step error of the trapezoidal method on this problem is $\mathcal{O}(k^3)$.

Solution.
a. We have that the trapezoidal method is given by

$$U^{n+1} = U^n + \frac{k}{2}(f(U^n) + f(U^{n=1}))$$

Using $u' = \lambda u = f(u)$, we see that

$$\begin{aligned} U^{n+1} &= U^n + \frac{k}{2}(\lambda U^n + \lambda U^{n+1}) \\ &= U^n + \frac{k\lambda}{2}U^n + \frac{k\lambda}{2}U^{n+1} \\ & U^n \frac{z}{2}U^n + \frac{z}{2}U^{n+1} \end{aligned}$$

Hence,

$$U^{n+1} - \frac{z}{2}U^{n+1} = U^n + \frac{z}{2}U^n$$

Therefore,

$$(1 - \frac{z}{2})U^{n+1} = (1 + \frac{z}{2})U^n$$

Thus,

$$U^{n+1} = (\frac{1 + z/2}{1 - z/2})U^n$$

as desired.

b. Let $R(Z)$ be as given above. Note that the Taylor series expansion of e^z about 0 is $e^z = 1 + z + \frac{z^2}{2} + \ldots$. Now, we are given the Neumann series $\frac{1}{1-z/2} = 1 + \frac{z}{2} + \frac{z^2}{4} + \frac{z^3}{8} + \ldots$. So,

$$R(z) = (1 + z/2)(\frac{1}{1 - z/2}) = (1 + z/2)(1 + \frac{z}{2} + \frac{z^2}{4} + \frac{z^3}{8} + \ldots)$$
$$= 1 + \frac{z}{2} + \frac{z}{2} + \frac{z^2}{4} + \frac{z^2}{4} + \frac{z^3}{8} + \frac{z^3}{8} + \ldots$$
$$= 1 + z + \frac{z^2}{2} + \mathcal{O}(z^3) = e^z + \mathcal{O}(z^3)$$

Hence, we see that the one-step error of the trapezoidal method on this problem is $\mathcal{O}(k^3)$ as desired.