1. Implicit and explicit analogues of common methods [20 points]

There are two classes of methods for the problem $du/dt = a(u(t))$ that were not discussed much in class; implicit Runge-Kutta methods and explicit analogs of Backward Differentiation formulas.

(a) Consider the two-stage implicit Runge-Kutta method given by

$$u^{n+1} = u^n + \Delta t\left(\frac{1}{2}k_1 + \frac{1}{2}k_2\right)$$
$$k_1 = a\left(u^n + \frac{\Delta t}{4}k_1 + \Delta t\left(\frac{1}{4} - \frac{\sqrt{3}}{6}\right)k_2\right)$$
$$k_2 = a\left(u^n + \Delta t\left(\frac{1}{4} + \frac{\sqrt{3}}{6}\right)k_1 + \frac{\Delta t}{4}k_2\right).$$

Determine and plot the linear stability diagram of this scheme. Given this stability, why would this *fouth-order* scheme not be used in practice?

(b) Explicit analogues of the Backward Differentiation Formulas have the general form

$$u^{n+1} + \sum_{i=0}^{S}\alpha_i u^{n-i} = \beta f(u^n).$$

Derive the second-order and third-order methods of this form and determine and plot their linear stability characteristics. What is the second-order method? Would you ever want to use these methods in practice? (*Hint: Be very careful with your stability diagrams.*)

(a) $\frac{du}{dt} = a(u) = Au(t)$ for linear stability analysis

$$k_1 = Au^n + \frac{1}{4}\Delta t\, Ak_1 + \Delta t\left(\frac{1}{4} - \frac{\sqrt{3}}{6}\right)Ak_2$$

$$k_2 = Au^n + \Delta t\left(\frac{1}{4} + \frac{\sqrt{3}}{6}\right)Ak_1 + \frac{1}{4}\Delta t\, Ak_2$$

$$\left(1 - \frac{1}{4}\Delta t A\right)k_1 - \Delta t\left(\frac{1}{4} - \frac{\sqrt{3}}{6}\right)Ak_2 = Au^n$$

$$-\Delta t\left(\frac{1}{4} + \frac{\sqrt{3}}{6}\right)Ak_1 + \left(1 - \frac{1}{4}\Delta t A\right)k_2 = Au^n$$

$$\Rightarrow \begin{pmatrix} 1 - \frac{1}{4}\Delta t A & -\Delta t\left(\frac{1}{4} - \frac{\sqrt{3}}{6}\right)A \\ -\Delta t\left(\frac{1}{4} + \frac{\sqrt{3}}{6}\right)A & 1 - \frac{1}{4}\Delta t A \end{pmatrix}\begin{pmatrix} k_1 \\ k_2 \end{pmatrix} = \begin{pmatrix} Au^n \\ Au^n \end{pmatrix}$$

$$\begin{pmatrix} k_1 \\ k_2 \end{pmatrix} = \begin{pmatrix} 1 - \frac{1}{4}\Delta t A & -\Delta t\left(\frac{1}{4} - \frac{\sqrt{3}}{6}\right)A \\ -\Delta t\left(\frac{1}{4} + \frac{\sqrt{3}}{6}\right)A & 1 - \frac{1}{4}\Delta t A \end{pmatrix}^{-1}\begin{pmatrix} Au^n \\ Au^n \end{pmatrix}$$

Assume that the system is 1-D for convenience. then $A \to a$

$$\begin{pmatrix} k_1 \\ k_2 \end{pmatrix} = \frac{1}{\left(1-\frac{1}{4}\Delta t a\right)^2 - \Delta t^2 \cdot \left(\frac{1}{16}-\frac{1}{12}\right)a^2} \begin{pmatrix} 1-\frac{1}{4}\Delta t a & \Delta t\left(\frac{1}{4}-\frac{\sqrt{3}}{6}\right)a \\ \Delta t\left(\frac{1}{4}+\frac{\sqrt{3}}{6}\right)a & 1-\frac{1}{4}\Delta t a \end{pmatrix} \begin{pmatrix} a u^n \\ a u^n \end{pmatrix}$$

$$= \frac{1}{1-\frac{1}{2}\Delta t a + \frac{1}{12}\Delta t^2 a^2} \begin{pmatrix} a u^n - \frac{\sqrt{3}}{6} a^2 \Delta t \, u^n \\ \frac{\sqrt{3}}{6} a^2 \Delta t \cdot u^n + a u^n \end{pmatrix}$$

$$u^{n+1} = u^n + \frac{1}{2}\Delta t \cdot 2 a u^n \cdot \frac{1}{1-\frac{1}{2}\Delta t a + \frac{1}{12}\Delta t^2 a^2}$$

$$= u^n + \frac{a \Delta t \, u^n}{1-\frac{1}{2}\Delta t a + \frac{1}{12}\Delta t^2 \cdot a^2}$$

$$= \left(\frac{1+\frac{1}{2}\Delta t a + \frac{1}{12}\Delta t^2 a^2}{1-\frac{1}{2}\Delta t \cdot a + \frac{1}{12}\Delta t^2 a^2}\right) u^n$$

$$\left| \frac{1+\frac{1}{2}\Delta t a + \frac{1}{12}\Delta t^2 a^2}{1-\frac{1}{2}\Delta t a + \frac{1}{12}\Delta t^2 a^2} \right| < 1$$ is required for linear stability

Let $a\Delta t := z$ where $z = a_r \Delta t + i a_i \Delta t$ then

$$\left| \frac{1+\frac{1}{2}z + \frac{1}{12}z^2}{1-\frac{1}{2}z + \frac{1}{12}z^2} \right| < 1$$ corresponds to linear stability regime.

(5)

$$a^{n+1} + \sum_{i=0}^{s} \alpha_i a^{n-i} = \beta f(a^n)$$

(i) For second order.

$$a^{n+1} + \alpha_0 a^n + \alpha_1 a^{n-1} = \beta f(a^n)$$

(ii) For third order.

$$a^{n+1} + \alpha_0 a^n + \alpha_1 a^{n-1} + \alpha_2 a^{n-2} = \beta f(a^n)$$

(i) $\frac{da}{dt} \approx \frac{a^{n+1} - 4a^n + a^{n-1}}{2\Delta t} = f(a^n)$

$\Rightarrow$ $a^{n+1} - 4a^n + a^{n-1} = 2\Delta t f(a^n)$

$\alpha_0 = -4 \quad \alpha_1 = 1 \quad \beta = 2\Delta t$

Let $f(a^n) = a a^n$ then

$$a^{n+1} = (4 + 2a\Delta t)a^n - a^{n-1}$$

Let $\frac{a^{n+1}}{a^n} = \rho$ then $\frac{a^n}{a^{n-1}} = \rho$

$\rho = (4+2a\Delta t) - \frac{1}{\rho}$, $\rho^2 - (4+2a\Delta t)\rho + 1 = 0$

$\rho = (2+a\Delta t) \pm \sqrt{(2+a\Delta t)^2 - 1}$, let $a\Delta t := z$

$\rho = (2+z) \pm \sqrt{(2+z)^2 - 1}$

linear stability regime : $|\rho| \leq 1$, $\left| 2+z \pm \sqrt{(2+z)^2-1} \right| \leq 1$

(iii) $\frac{da}{dt} = \frac{11a^{n+1} - 18a^n + 9a^{n-1} - 2a^{n-2}}{6\Delta t} = f(a^n)$

$11a^{n+1} - 18a^n + 9a^{n-1} - 2a^{n-2} = 6\Delta t \, f(a^n)$

$a^{n+1} = \left(\frac{18}{11} + 6\Delta t a\right)a^n - \frac{9}{11}a^{n-1} + \frac{2}{11}a^{n-2}$

let $\rho := \frac{a^{n+1}}{a^n}$, $\rho = \left(\frac{18}{11} + 6\Delta t a\right) - \frac{9}{11}\frac{1}{\rho} + \frac{2}{11}\frac{1}{\rho^2}$

$\rho^3 - \left(\frac{18}{11} + 6\Delta t a\right)\rho^2 + \frac{9}{11}\rho - \frac{2}{11} = 0$

$\Rightarrow \rho = \rho(z)$

3. Conserved energy for the Verlet scheme [15 points]

The undamped oscillator *without* forcing is given by the dynamical system

$$\frac{d^2x}{dt^2} + \omega^2 x = 0, \qquad (*)$$

with initial position $x(0) = x_0$ and velocity $v(0) = \dot{x}(0) = v_0$. In Lecture 16: Symplectic Integrators, the second-order Verlet scheme was presented. One may discover that the determinant of the Jacobian of the scheme for $\boxed{*}$ is trivially equal to one—which implies a conserved quantity. Observe the modified energy $\boxed{2}$

$$\hat{H} = \frac{1}{2}v^2 + \frac{1}{2}\omega^2 x^2 \left(1 - \frac{\omega^2(\Delta t)^2}{4}\right).$$

Show that $\hat{H}$ is conserved in the second-order Verlet scheme for the simple harmonic oscillator $\boxed{*}$.

The Verlet algorithm

$$v^{n+1/2} = v^n - w^2 x^n \cdot \tfrac{1}{2}\Delta t$$

$$x^{n+1} = x^n + v^{n+1/2} \cdot \Delta t$$

$$v^{n+1} = v^{n+1/2} - w^2 x^{n+1} \cdot \Delta t/2$$

$$\Rightarrow \quad x^{n+1} = x^n + (v^n - w^2 x^n \cdot \tfrac{1}{2}\Delta t) \cdot \Delta t$$

$$v^{n+1} = v^n - w^2 x^n \cdot \tfrac{1}{2}\Delta t - w^2 \left(x^n + \left\{ v^n - w^2 x^n \cdot \tfrac{1}{2}\Delta t \right\} \cdot \Delta t \right) \cdot \tfrac{1}{2}\Delta t$$

$$x^{n+1} = x^n \cdot (1 - \tfrac{1}{2}w^2 \cdot \Delta t^2) + v^n \cdot \Delta t$$

$$v^{n+1} = v^n \cdot (1 - \tfrac{1}{2}w^2 \cdot \Delta t^2) - x^n \cdot (w^2 \Delta t - w^4 \cdot \tfrac{1}{4}\Delta t^3)$$

$$\begin{pmatrix} x^{n+1} \\ v^{n+1} \end{pmatrix} = \underbrace{\begin{pmatrix} 1 - \frac{1}{2}w^2\Delta t^2, & \Delta t \\ -w^2\Delta t + \frac{1}{4}w^4\Delta t^3, & 1 - \frac{1}{2}w^2\Delta t^2 \end{pmatrix}}_{A} \begin{pmatrix} x^n \\ v^n \end{pmatrix}$$

$$H = \tfrac{1}{2}w^2x^2 + \tfrac{1}{2}v^2 \quad \Rightarrow \quad \frac{\partial H}{\partial v} = v \qquad \frac{\partial H}{\partial x} = -\dot{v} = wx$$

$$\det A = (1 - \tfrac{1}{2}w^2\Delta t^2)^2 - \Delta t(-w^2\Delta t + \tfrac{1}{4}w^4\Delta t^3) = 1$$

$$\hat{H} = \tfrac{1}{2}[x, v] \underbrace{\begin{bmatrix} w^2(1 - \frac{1}{4}w^2\Delta t^2) & 0 \\ 0 & 1 \end{bmatrix}}_{M} \begin{bmatrix} x \\ v \end{bmatrix}$$

$$\hat{H}(x_{n+1}, v_{n+1}) = \frac{1}{2}(x_{n+1}\ \ v_{n+1})\, M \begin{pmatrix} x_{n+1} \\ v_{n+1} \end{pmatrix} = \frac{1}{2}(x_n\ \ v_n)\, A^T M A \begin{pmatrix} x_n \\ v_n \end{pmatrix}$$

If $A^T M A = M$ then $\hat{H}(x_{n+1}, v_{n+1}) = \hat{H}(x_n, v_n)$ thus conserved

$$A = \begin{pmatrix} 1 - \frac{1}{2}\omega^2 \Delta t^2 & \Delta t \\ -\omega^2 \Delta t + \frac{1}{4}\omega^4 \Delta t^3 & 1 - \frac{1}{2}\omega^2 \Delta t^2 \end{pmatrix} = \begin{pmatrix} 1 - \frac{1}{2}\omega^2 \Delta t^2 & \Delta t \\ -\omega^2 \Delta t (1 - \frac{1}{4}\omega^2 \Delta t^2) & 1 - \frac{1}{2}\omega^2 \Delta t^2 \end{pmatrix}$$

$$A^T M A = \begin{pmatrix} 1 - \frac{1}{2}\omega^2 \Delta t^2 & -\omega^2 \Delta t (1 - \frac{1}{4}\omega^2 \Delta t^2) \\ \Delta t & 1 - \frac{1}{2}\omega^2 \Delta t^2 \end{pmatrix} \begin{pmatrix} \omega^2 (1 - \frac{1}{4}\omega^2 \Delta t^2) & 0 \\ 0 & 1 \end{pmatrix} A$$

$$= \begin{pmatrix} (1 - \frac{1}{2}\omega^2 \Delta t^2)(1 - \frac{1}{4}\omega^2 \Delta t^2)\omega^2 & -\omega^2 \Delta t (1 - \frac{1}{4}\omega^2 \Delta t^2) \\ \omega^2 \Delta t (1 - \frac{1}{4}\omega^2 \Delta t^2) & 1 - \frac{1}{2}\omega^2 \Delta t^2 \end{pmatrix} \begin{pmatrix} 1 - \frac{1}{2}\omega^2 \Delta t^2 & \Delta t \\ -\omega^2 \Delta t (1 - \frac{1}{4}\omega^2 \Delta t^2) & 1 - \frac{1}{2}\omega^2 \Delta t^2 \end{pmatrix}$$

$$= \begin{bmatrix} (1 - \frac{1}{2}\omega^2 \Delta t^2)^2 (1 - \frac{1}{4}\omega^2 \Delta t^2)\omega^2 + \omega^4 \Delta t^2 (1 - \frac{1}{4}\omega^2 \Delta t^2)^2 & 0 \\ 0 & (1 - \frac{1}{2}\omega^2 \Delta t^2)^2 + \omega^2 \Delta t^2 (1 - \frac{1}{4}\omega^2 \Delta t^2) \end{bmatrix}$$

$$= \begin{bmatrix} \omega^2 (1 - \frac{1}{4}\omega^2 \Delta t^2) \left\{ (1 - \frac{1}{2}\omega^2 \Delta t^2)^2 + \omega^2 \Delta t^2 (1 - \frac{1}{4}\omega^2 \Delta t^2) \right\} & 0 \\ 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} \omega^2 (1 - \frac{1}{4}\omega^2 \Delta t^2) & 0 \\ 0 & 1 \end{bmatrix} = A$$

Therefore $\hat{H}(x_{n+1}, v_{n+1}) = \hat{H}(x_n, v_n)$ so it is conserved.