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AST 560; HW1

1. $x'(t) = \lambda x(t) + g(t)$; $0 < t < t_f$

and; $x(0) = 0$

Now; $x(t_n + h) = x(t_n) + h\,x'(t_n) + \frac{h^2}{2!} x''(t_n) + \underbrace{T_{n+1}}_{O(h^3)}$.

Now; $x'(t_n) = \lambda x(t_n) + g(t_n)$

$x''(t_n) = \lambda x'(t_n) + g'(t_n)$.

$= \lambda^2 x(t_n) + \lambda g(t_n) + g'(t_n)$.

So, $x(t_n+h) = x(t_n) + h\left(\lambda x(t_n) + g(t_n)\right) + \frac{h^2}{2}\left[\lambda^2 x(t_n) + \lambda g(t_n) + g'(t_n)\right] + \underbrace{O(h^3)}_{T_{n+1}}$

$$\Rightarrow \boxed{x(t_n+h) = \frac{\lambda^2 h^2}{2} x(t_n) + \lambda h x(t_n) + x(t_n) + h\left[\frac{\lambda h}{2} g(t_n) + g(t_n) + \frac{h}{2} g'(t_n)\right] + T_{n+1}}$$

Now; $\cancel{x_{n+1}} = x'_n = \lambda x_n + g(t_n)$ (from IVP)

So, $z(t_n+h) = z(t_n) + h z'(t_n) + \frac{h^2}{2} z''(t_n) \equiv TS(2)$ (Ignoring terms above order $O(h^2)$)

$\downarrow TS(2)$

$x_{n+1} = x_n + h x'_n + \frac{h^2}{2} x''_n$

Now, $x'_n = \lambda x_n + g(t_n)$

and; $x''_n = \lambda x'_n + g'(t_n) = \lambda(\lambda x_n + g(t_n)) + g'(t_n)$

So, $\boxed{x_{n+1} = x_n + h(\lambda x_n + g(t_n)) + \frac{h^2}{2}\left[\lambda^2 x_n + \lambda g(t_n) + g'(t_n)\right]}$

To check the global error for TS(2):-

GE = Exact soln − Discretized to $O(h^2)$ accuracy.

so; $|x(t_n+h) - x_{n+1}|$

$$\leq |x(t_n) - x_n| + \lambda h\,|x(t_n) - x_n| + \frac{\lambda^2 h^2}{2}\,|x(t_n) - x_n| + 0 + T_{n+1}$$

the $g(t_n)$ and $g'(t_n)$ terms cancel out.

$$\Rightarrow e_{n+1} \leq e_n + \lambda h\, e_n + \frac{(\lambda h)^2}{2} e_n + T_{n+1}$$

$$\Rightarrow e_{n+1} \leq \left\{1 + \lambda h + \frac{(\lambda h)^2}{2!}\right\} e_n + T_{n+1}$$

Now; from Maclaurin expansion we know that:-

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots$$

$$\Rightarrow e^x \geq 1 + x + \frac{x^2}{2!} \Rightarrow 1 + \lambda h + \frac{(\lambda h)^2}{2!} \leq e^{\lambda h}$$

so; $\boxed{e_{n+1} \leq \{\exp(\lambda h)\} e_n + T_{n+1}}$

Now; <u>using recursion</u>:-

$$e_1 = \{\exp(\lambda h)\} e_0 + T_1$$

$$e_2 = \{\exp(\lambda h)\}^2 e_0 + \exp(\lambda h) T_1 + T_2$$

$$\vdots$$

$$e_n = \{\exp(\lambda h)\}^n e_0 + \sum_{j=1}^{n} \{\exp(\lambda h)\}^{n-j} T_j$$

$$= \left(e^{n\lambda h}\right) e_0 + \sum_{j=1}^{n} \exp\left(\overline{n-j}\,\lambda h\right) T_j$$

Now; e_0 = initial error $= 0$ as the initial value does not suffer from any truncation error.

So;
$$e_n \leq \sum_{j=1}^{n} \exp(\overline{n-j}\,\lambda h)\, T_j$$

Now, $\exp(\overline{n-j}\,\lambda h) \leq \exp(n\lambda h)$

So;
$$e_n \leq \sum_{j=1}^{n} \exp(n\lambda h)\, T_j$$

and $T_j \leq ch^3$

c → some constant factor

h^3 → as the truncation error is of order $O(h^3)$

So; $e_n \leq nch^3 e^{n\lambda h}$

Now; $nh = T_f$ → time of simulation

So;
$$\boxed{e_n \leq cT_f h^2 e^{\lambda T_f}}$$

So; G.E $\sim O(h^2)$ whereas LE $\sim O(h^3)$.

which can be generalized similarly to TS(p) where GE $\sim O(h^p)$ and LE $\sim O(h^{p+1})$.

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3. Let us apply this to the IVP

$$x'(t) = \lambda x(t).$$

so; $f_{n+1} = x'(t_{n+1}) = x'_{n+1} = \lambda x_{n+1}$

2. $x_{n+2} - x_n = 2hf_{n+1}$

$P(r) = r^2 - 1 - 2h\lambda r$

$\Rightarrow r^2 - 2\hat{h}r - 1.$ $\qquad \hat{h} = h\lambda$

where $Re(\lambda) < 0.$

so, $Re(\hat{h}) < 0.$

so, $P(r) = r^2 - 2\hat{h}r - 1 = 0$

$\downarrow$

roots $= r_{\pm} = \dfrac{+2\hat{h} \pm \sqrt{4\hat{h}^2 + 4.1}}{2}$

$$\boxed{r_{\pm} = \hat{h} \pm \sqrt{\hat{h}^2 + 1}}$$

$|r_{\pm}| < 1 \Rightarrow |r_{\pm}|^2 < 1$

$\cancel{\Rightarrow |\hat{h}|^2 + |\hat{h}|^2 + 1 \pm 2\hat{h}\sqrt{|\hat{h}|^2 + 1} < 1}$

Let; $\hat{h} = \hat{h}_r + i\hat{h}_i$

$\cancel{\text{so, } |r_-|^2 = \hat{h}_r^2 + \hat{h}_i^2 + \hat{h}_r^2 + \hat{h}_i^2 + 1 - 2h_r}$

$|r_-|^2 = (h_r - \sqrt{h_r^2 + h_i^2 + 1})^2 + h_i^2$

$\Rightarrow h_r^2 + h_r^2 + h_i^2 + 1 - 2h_r\sqrt{h_r^2 + h_i^2 + 1} + h_i^2$

$\Rightarrow 2(h_r^2 + h_i^2) + 1 - 2h_r\sqrt{h_r^2 + h_i^2 + 1}$

so, $|r_-|^2 > 1$ if $h_r < 0$

and we know $h_r < 0$ as $Re(\lambda) < 0$ and $h > 0.$

so, nowhere in our $\hat{h}$ complex plane is $|r_-| < 1$

as whenever $h_r < 0$ (which is everywhere); $|r_-| > 1.$

So, no region of absolute stability.

3. <u>IVP:</u> $x'(t)=1$ and $x(0)=0$

$$x_{n+1} = x_n + h\sum_{i=1}^{s} b_i k_i$$

$$\text{and } k_i = f\left(t_n + c_i h,\ x_n + h\sum_{j=1}^{s} a_{i,j} k_j\right)$$

$$= f(t_n, x_n) + O(h)$$

$$\text{so: } \boxed{x_{n+1} = x_n + h\sum_{i=1}^{s} b_i f(t_n, x_n) + O(h^2).}$$

To converge; the algorithm atleast needs to be consistent. ~~Here; only 1st order derivative is specified~~

Now, $x(t_n+h) = x(t_n) + h f(x_n, t_n) + O(h^2)$

$$\text{so: } x(t_n+h) - x_{n+1} = x(t_n) - x_n + h\left(\sum_{j=1}^{s} b_j - 1\right) f(x_n, t_n) + O(h^2)$$

Assuming $x(t_n) = x_n$ (localization assumption);

$$T_{n+1} = h\left(\sum_{j=1}^{s} b_j - 1\right) f(x_n, t_n) + O(h^2)$$

so; for being atleast first order accurate; (so that the $x'(t)=1$ derivate can be implemented accurately); we need the coefficient of $O(h)$ to vanish everywhere

$$\Rightarrow \left(\sum_{j=1}^{s} b_j - 1\right) = 0$$

$$\Rightarrow \boxed{\sum_{j=1}^{s} b_j = 1}$$

Or, we could do it for the very first step's exact solution:

$x'(t) = 1 \Rightarrow \cancel{x(t) = t}$

$$\Rightarrow \int \frac{dx}{dt}\, dt = \int dt \rightarrow x(t) - x(0) = t$$

So, $x(h) - x(0) = h \Rightarrow x(h) = x(0) + h$
$= h$

as $\boxed{x(0) = 0}$

so, $x(h) = h$ (exact soln)

Now, $$x_{n+1} = x_n + h \sum_{i=1}^{s} b_i f(t_n, x_n)$$

$$x_1 = \underset{\downarrow\, 0}{x_0} + h \sum_{i=1}^{s} b_i \underbrace{f(t_0, x_0)}_{x'(t_0, x_0) = 1} + O(h^2)$$

$$\Rightarrow x_1 = h \sum_{i=1}^{s} b_i + O(h^2).$$

$$\Rightarrow x(h) = h$$

So, $$x(h) - x_1 = h\left(1 - \sum_{j=1}^{s} b_j\right) + O(h^2)$$

So, for converging; LTE $\sim O(h^2)$; i.e., it has to be consistent of order 1.

So, $$1 - \sum_{j=1}^{s} b_j = 0 \Rightarrow \boxed{\sum_{j=1}^{s} b_j = 1}$$

4. Given: $\Phi: Z_0 \longmapsto Z_1$ and $\Psi: Z_1 \longrightarrow Z_2$ are symplectic maps.

So, let M_{01} be the symplectic matrix for Φ

and M_{12} be the symplectic matrix for Ψ.

Also, let M_{02} be the symplectic matrix for $(\Psi \circ \Phi) = \varphi: Z_0 \longrightarrow Z_2$

given that :- $M_{01}^T J M_{01} = J$ and $M_{12}^T J M_{12} = J$

so; $M_{02}^T J M_{02} = ?$

$$\cancel{= M_{02}^T M_{12}^T J M_{12} M_{02}}$$

Now; $M_{01} = \begin{pmatrix} \frac{\partial q_1}{\partial q_0} & \frac{\partial q_1}{\partial p_0} \\ \frac{\partial p_1}{\partial q_0} & \frac{\partial p_1}{\partial p_0} \end{pmatrix}$ and $M_{12} = \begin{pmatrix} \frac{\partial q_2}{\partial q_1} & \frac{\partial p_2}{\partial p_1} \\ \frac{\partial p_2}{\partial q_1} & \frac{\partial p_2}{\partial p_1} \end{pmatrix}$

and; $M_{02} = \begin{pmatrix} \frac{\partial q_2}{\partial q_0} & \frac{\partial q_2}{\partial p_0} \\ \frac{\partial p_2}{\partial q_0} & \frac{\partial p_2}{\partial p_0} \end{pmatrix}$.

Now; as q_2 depends on q_1 and p_1 as well;

$$\frac{\partial q_2}{\partial q_0} = \frac{\partial q_2}{\partial q_1}\frac{\partial q_1}{\partial q_0} + \frac{\partial q_2}{\partial p_1}\frac{\partial p_1}{\partial q_0} \quad \text{(by chain rule)}.$$

so; similarly;

$$M_{02} = \begin{pmatrix} \frac{\partial q_2}{\partial q_1}\frac{\partial q_1}{\partial q_0} + \frac{\partial q_2}{\partial p_1}\frac{\partial p_1}{\partial q_0} & \frac{\partial q_2}{\partial q_1}\frac{\partial q_1}{\partial p_0} + \frac{\partial q_2}{\partial p_1}\frac{\partial p_1}{\partial p_0} \\ \frac{\partial p_2}{\partial q_1}\frac{\partial q_1}{\partial q_0} + \frac{\partial p_2}{\partial p_1}\frac{\partial p_1}{\partial q_0} & \frac{\partial p_2}{\partial q_1}\frac{\partial q_1}{\partial p_0} + \frac{\partial p_2}{\partial p_1}\frac{\partial p_1}{\partial p_0} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{\partial q_2}{\partial q_1} & \frac{\partial q_2}{\partial p_1} \\ \frac{\partial p_2}{\partial q_1} & \frac{\partial p_2}{\partial p_1} \end{pmatrix}\begin{pmatrix} \frac{\partial q_1}{\partial q_0} & \frac{\partial q_1}{\partial p_0} \\ \frac{\partial p_1}{\partial q_0} & \frac{\partial p_1}{\partial p_0} \end{pmatrix} = M_{12} M_{01}$$

so; $M_{02} = M_{12} M_{01}$

so; $M_{02}^T J M_{02} = (M_{12} M_{01})^T J (M_{12} M_{01})$

$$= M_{01}^T (M_{12}^T J M_{12}) M_{01}$$

$$= M_{01}^T J M_{01} = J$$

so; $\boxed{M_{02}^T J M_{02} = J}$ Hence; $\psi \circ \phi : Z_0 \longrightarrow Z_2$ is also a symplectic map!

5. Semi-implicit Euler's

$$\left.\begin{array}{l} p_{n+1} = p_n - h H_q (p_{n+1}, q_n) \\ q_{n+1} = q_n + h H_p (p_{n+1}, q_n) \end{array}\right\} \text{ Implicit in } p.$$

Here; we have $H(\bar{q}, \bar{p}) = \frac{1}{2}\left[\bar{p} - \bar{A}(\bar{q})\right]^2 + \phi(\bar{q})$

and Linear in p $\longrightarrow \frac{\partial H}{\partial p_i} = \{p_i - A_i(q)\}$ ~~and $\frac{\partial H}{\partial q_i} = -2 \frac{\partial A_i}{\partial q_i} + \frac{\partial \phi}{\partial q_i}$~~

and Non-lin in q $\longrightarrow \frac{\partial H}{\partial q_i} = \left\{ -\left[\bar{p} - \bar{A}(\bar{q})\right]_j \frac{\partial A_j}{\partial q_i} + \frac{\partial \phi}{\partial q_i} \right\}$ (much more complicated & non-linear)

Now, if we do an implicit in q; the would mean we would have to evaluate $\frac{\partial H}{\partial q_i}(q_{n+1}, p_n)$ and ~~therefore~~; ~~solve a matrix eq~~ so; we would end up with a possibly non-linear equation in q_{n+1} which is coupled in time.

However; if we choose p as the implicit dimension; the problem is much simple as $H_p = p$ and so linear and therefore; would give as a solvable matrix equation.

So, for the given hamiltonian; we should solve with p as the implicit variable.

6. $\dot{z} = J \nabla H$

and $\dfrac{z^{n+1} - z^n}{h} = J \nabla H \Big|_{(z^{n+1}+z^n)/2}$

So, $q^{n+1} = q^n + h H_p$ evaluated at $\left(\dfrac{z^{n+1}+z^n}{2}\right)$.

and, $p^{n+1} = p^n - h H_q$

Now, $\dfrac{\partial q^{n+1}}{\partial q^n} = 1 + h \dfrac{\partial H_p}{\partial q^n}\Big|_{\left(\frac{z^{n+1}+z^n}{2}\right)}$ ~~$= 1 + h\, \partial H_p$~~

Now $\dfrac{\partial H_p}{\partial q^n}\Big|_{\frac{z^{n+1}+z^n}{2}} = H_{pq}\left(\dfrac{\frac{\partial q^{n+1}}{\partial q^n} + \frac{\partial q^n}{\partial q^n}}{2}\right) + H_{pp}\left(\dfrac{\frac{\partial p^{n+1}}{\partial q^n} + \frac{\partial p^n}{\partial q^n}}{2}\right)$

$\Rightarrow H_{pp}\left(\dfrac{\frac{\partial p^{n+1}}{\partial q^n}}{2}\right) + H_{pq}\left(\dfrac{\frac{\partial q^{n+1}}{\partial q^n} + 1}{2}\right).$

So, $\boxed{\dfrac{\partial q^{n+1}}{\partial q^n} = 1 + \dfrac{h}{2} H_{pp}\left(\dfrac{\partial p^{n+1}}{\partial q^n}\right) + \dfrac{h}{2} H_{pq}\left(\dfrac{\partial q^{n+1}}{\partial q^n} + 1\right)}$

Now similarly;

$\Rightarrow \dfrac{\partial q^{n+1}}{\partial p^n} = 0 + \dfrac{h}{2} H_{pq}\left(\dfrac{\partial q^{n+1}}{\partial p^n}\right) + \dfrac{h}{2} H_{pp}\left(\dfrac{\partial p^{n+1}}{\partial p^n} + 1\right).$

$\Rightarrow \dfrac{\partial p^{n+1}}{\partial q^n} = 0 - \dfrac{h}{2} H_{qq}\left(\dfrac{\partial q^{n+1}}{\partial q^n} + 1\right) - \dfrac{h}{2} H_{qp}\left(\dfrac{\partial p^{n+1}}{\partial q^n}\right)$

$\Rightarrow \dfrac{\partial p^{n+1}}{\partial p^n} = 1 - \dfrac{h}{2} H_{qq}\left(\dfrac{\partial q^{n+1}}{\partial p^n}\right) - \dfrac{h}{2} H_{qp}\left(\dfrac{\partial p^{n+1}}{\partial p^n} + 1\right)$

So; constructing $M = \begin{pmatrix} \frac{\partial q^{n+1}}{\partial q^n} & \frac{\partial q^{n+1}}{\partial p^n} \\ \frac{\partial p^{n+1}}{\partial q^n} & \frac{\partial p^{n+1}}{\partial p^n} \end{pmatrix}$

$$\Rightarrow \begin{bmatrix} 1 + \frac{h}{2} H_{pq}\left(\frac{\partial q^{n+1}}{\partial p^n}\right) + \frac{h}{2} H_{pp}\left(\frac{\partial p^{n+1}}{\partial p^n} + 1\right) & \frac{h}{2} H_{pq}\left(\frac{\partial q^{n+1}}{\partial p^n}\right) + \frac{h}{2} H_{pp}\left(\frac{\partial p^{n+1}}{\partial p^n} + 1\right) \\ -\frac{h}{2} H_{qq}\left(\frac{\partial q^{n+1}}{\partial q^n} + 1\right) - \frac{h}{2} H_{qp}\left(\frac{\partial p^{n+1}}{\partial q^n}\right) & 1 - \frac{h}{2} H_{qq}\left(\frac{\partial q^{n+1}}{\partial p^n}\right) - \frac{h}{2} H_{qp}\left(\frac{\partial p^{n+1}}{\partial p^n} + 1\right) \end{bmatrix}$$

$\downarrow$ can be recast into

$$\begin{pmatrix} 1 - \frac{h}{2} H_{pq} & -\frac{h}{2} H_{pp} \\ \frac{h}{2} H_{qq} & 1 + \frac{h}{2} H_{qp} \end{pmatrix} \begin{pmatrix} \frac{\partial q^{n+1}}{\partial q^n} & \frac{\partial q^{n+1}}{\partial p^n} \\ \frac{\partial p^{n+1}}{\partial q^n} & \frac{\partial p^{n+1}}{\partial p^n} \end{pmatrix} \longrightarrow M$$

$$= \begin{pmatrix} \frac{h}{2} H_{pq} + 1 & \frac{h}{2} H_{pp} \\ -\frac{h}{2} H_{qq} & 1 - \frac{h}{2} H_{pq} \end{pmatrix}$$

so; let $1 - \frac{h}{2} H_{pq} = a$; $-\frac{h}{2} H_{pp} = b$, $\frac{h}{2} H_{qq} = c$,

$1 + \frac{h}{2} H_{pq} = d$

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} M = \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

Now;
$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

$$= \frac{1}{ad - bc} \begin{pmatrix} +d & -c \\ -b & +a \end{pmatrix}^{T} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

$$\Rightarrow M = \frac{1}{ad-bc}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

So, let $A = \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$

So, $M = \frac{1}{|A|} AA$ where $|A| = \det(A)$

Now, $M^T J M = \frac{1}{|A|^2} A^T A^T J A A$

Now, $A^T J A = \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}^T \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$

$$\Rightarrow \begin{pmatrix} d & -c \\ -b & a \end{pmatrix}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} c & d \\ -a & -b \end{pmatrix}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix} = \begin{pmatrix} \cancel{cd} - \cancel{cd} & -bc+ad \\ -ad+bc & \cancel{ab} - \cancel{ab} \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} 0 & ad-bc \\ -(ad-bc) & 0 \end{pmatrix} = |A|\, J$$

So, $A^T J A = |A| J$

$$\Rightarrow M^T J M = \frac{1}{|A|^2} A^T (A^T J A) A$$

$$\Rightarrow \frac{|A|}{|A|^2} (A^T J A) = \frac{|A|^2}{|A|^2} J = J$$

So, $\boxed{M^T J M = J}$. Hence, map is symplectic.