Lecture 8

Paul Andries Zegeling

Department of Mathematics, Utrecht University

Numerical Methods for Time-Dependent PDEs, Spring 2024

Outline of Lecture 8

- Hamiltonian ODEs
- Hamiltonian PDEs

Hamiltonian ODEs [1]

General linear 2x2 ODE-system:

$$\begin{cases} x' = ax + by \\ y' = cx + dy \end{cases} \qquad A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

$$\lambda_1, \lambda_2 \; ; \; \lambda_1 \neq \lambda_2$$

an exact FD-scheme:

$$\begin{cases} \dfrac{x^{n+1} - \psi x^n}{\phi} = a x^n + b y^n \\[2ex] \dfrac{y^{n+1} - \psi y^n}{\phi} = c x^n + d y^n \end{cases} \quad \text{with} \quad \begin{cases} \phi = \dfrac{e^{\lambda_1 \Delta t} - e^{\lambda_2 \Delta t}}{\lambda_1 - \lambda_2} \\[2ex] \psi = \dfrac{\lambda_1 e^{\lambda_2 \Delta t} - \lambda_2 e^{\lambda_1 \Delta t}}{\lambda_1 - \lambda_2} \end{cases}$$

Special case: $\begin{cases} x' = y \\ y' = -x \end{cases} \qquad \lambda_{1,2} = \pm i$

an exact FD-scheme:

$$\begin{cases} \dfrac{x^{n+1} - x^n}{\phi} = \dfrac{y^{n+1} + y^n}{2} \\[2ex] \dfrac{y^{n+1} - y^n}{\phi} = -\dfrac{x^{n+1} + x^n}{2} \end{cases} \quad \text{with } \phi = \frac{2\,(1 - \cos(\Delta t))}{\Delta t \cdot \sin(\Delta t)}$$

$$\overset{!}{\Longrightarrow} \mathcal{H}^{n+1} = \mathcal{H}^n \quad \forall n \geq 0$$

(conservation of energy)

Hamiltonian ODEs [2]

$$\begin{cases} \dot{p} = -\dfrac{\partial \mathcal{H}}{\partial q}(p,q) \\ \dot{q} = \dfrac{\partial \mathcal{H}}{\partial p}(p,q) \end{cases}$$

$p = (p_1, p_2, \ldots, p_d)$

$q = (q_1, q_2, \ldots, q_d)$

$$\mathcal{H}(\underbrace{p_1, p_2, \ldots, p_d}_{\text{momenta}}, \underbrace{q_1, q_2, \ldots, q_d}_{\text{positions}})$$

"total energy"
"Hamiltonian" of the system

$d = \#$ degrees of freedom

- molecular dynamics (many particles)
- celestial mechanics (solar system)
- classical mechanics

Hamiltonian ODEs [3]

example
$d=1 \quad \mathcal{H}=\mathcal{H}(p,q)$

$$\frac{d\mathcal{H}}{dt} \underset{\uparrow}{=} \frac{\partial \mathcal{H}}{\partial p}\cdot \dot{p} + \frac{\partial \mathcal{H}}{\partial q}\cdot \dot{q} = \frac{\partial \mathcal{H}}{\partial p}\cdot -\frac{\partial \mathcal{H}}{\partial q} + \frac{\partial \mathcal{H}}{\partial q}\cdot\frac{\partial \mathcal{H}}{\partial p} = 0$$

chainrule

$\Rightarrow \mathcal{H}(p,q) = \text{constant}$
(energy is preserved)
in the time-direction

---

mathematical pendulum ($m=1$, $\ell=1$)
"$g=1$"

$$\mathcal{H}(p,q) = \frac{1}{2}p^2 - \cos(q) \Rightarrow \begin{cases} \dot{p} = -\sin(q) \\ \dot{q} = p \end{cases}$$

~ "$q=x$", "$p=y$" –

Hamiltonian ODEs [4]

special case: $\dot{x} = y, \; \dot{y} = -x$

$\sin(x) \approx x$ (small angles x)

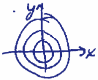
$\boxed{\text{EF}}$ $\begin{cases} x^{n+1} = x^n + h y^n \\ y^{n+1} = y^n - h x^n \end{cases}$ $(h = \Delta t)$

- conditionally stable
- first order

energy $= \mathcal{H} = \frac{1}{2} x^2 + \frac{1}{2} y^2$

$\mathcal{H} = \text{constant} : \; \frac{1}{2} x^2 + \frac{1}{2} y^2 = c^2$ circles

- t varies on each circle
- ICs determine which circle



discrete Hamiltonian $\underset{(\text{at } t = t^{n+1})}{\mathcal{H}^{n+1}} = \frac{1}{2}\left((x^{n+1})^2 + (y^{n+1})^2 \right)$

$= \text{----}$ (exercise)

$= \underbrace{\text{....}}_{>1} * \mathcal{H}^n > \underset{(\text{at } t = t^n)}{\mathcal{H}^n}$

Hamiltonian ODEs [5]

$\boxed{EB}$

- always stable
- first order

$$\begin{cases} x^{n+1} = x^n + h y^{n+1} \\ y^{n+1} = y^n - h x^{n+1} \end{cases}$$

$$\Rightarrow \begin{cases} x^{n+1} = x^n + h\left(y^n - h x^{n+1}\right) \Rightarrow x^{n+1} = \dfrac{x^n + h y^n}{1+h^2} \\ y^{n+1} = y^n - h\left(x^n + h y^{n+1}\right) \Rightarrow y^{n+1} = \dfrac{y^n - h x^n}{1+h^2} \end{cases}$$

discrete Hamiltonian: $\mathcal{H}^{n+1} = ---$

$= $ (exercise)

$$= \underbrace{---}_{<1} \cdot \mathcal{H}^n < \mathcal{H}^n$$

Hamiltonian ODEs [6]

implicit midpoint

$$\begin{cases} x^{n+1} = x^n + \frac{h}{2}(y^n + y^{n+1}) \\ y^{n+1} = y^n - \frac{h}{2}(x^n + x^{n+1}) \end{cases}$$

re-write

$$\Rightarrow \underbrace{\begin{pmatrix} 1 & -\frac{h}{2} \\ \frac{h}{2} & 1 \end{pmatrix}}_{\det = 1 + \frac{h^2}{4}} \begin{pmatrix} x^{n+1} \\ y^{n+1} \end{pmatrix} = \begin{pmatrix} x^n + \frac{h}{2} y^n \\ y^n - \frac{h}{2} x^n \end{pmatrix}$$

$$\overset{\cdots}{\Longrightarrow} \mathcal{H}^{n+1} = \overset{?}{\cdots} \times \mathcal{H}^n$$

exercise

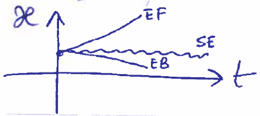
Hamiltonian ODEs [7]

Symplectic Euler

$\boxed{SE}$ $\begin{cases} x^{n+1} = x^n + h\, y^{n+1} \\ y^{n+1} = y^n - h \sin(x^n) \end{cases} \underset{\text{re-write}}{\Rightarrow} \begin{cases} y^{n+1} = y^n - h \sin(x^n) \\ x^{n+1} = x^n + h\left(y^n - h\sin(x^n)\right) \end{cases}$

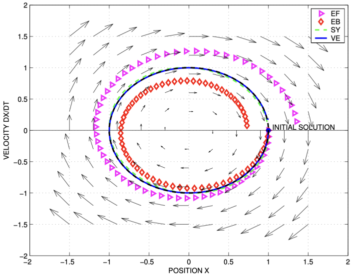
"implicit-explicit" "explicit"

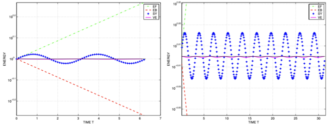
$\Rightarrow x^{n+1} \neq$ constant



Hamiltonian ODEs [8]

Phase plane solutions and the Hamiltonian (total energy):





Hamiltonian PDEs [1]

$\boxed{\dfrac{\delta}{\delta u}}$ variational or Fréchet derivative

* spatial interval $[0, L]$
* V: space of "smooth" functions
* inner product: $\langle u, v \rangle = \int_0^L u(x)\, v(x)\, dx \quad , u, v \in V$
* assume periodic BCs : $u(0) = u(L)$ (and, if needed, $u_x(0) = u_x(L)$ etcetera)

- functional $\mathcal{F}[u] : V \to \mathbb{R}$ (integral of u and its spatial derivatives $u_x, u_{xx}, \ldots$)

  Example: $\mathcal{F}[u] = \int_0^L f(u, u_x, u_{xx})\, dx = \int_0^L (u u_{xx} - u_x^2)\, dx$

- $\dfrac{\delta \mathcal{F}}{\delta u}$ is defined in a "weak sense":

$$\left\langle \frac{\delta \mathcal{F}}{\delta u}, v \right\rangle = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left[\mathcal{F}[u + \varepsilon v] - \mathcal{F}[u] \right] \quad \forall v \in V$$

Hamiltonian PDEs [2]

<u>Example:</u> (1)

$$\mathcal{F}[u] = \int_0^L u^3\,dx \quad \Rightarrow \quad \mathcal{F}[u+\varepsilon v] = \int_0^L (u+\varepsilon v)^3\,dx$$

$$\Rightarrow \left\langle \frac{\delta \mathcal{F}}{\delta u}, v \right\rangle = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon}\left(\int_0^L (u+\varepsilon v)^3\,dx - \int_0^L u^3\,dx \right)$$

$$= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \int_0^L \left(\cancel{u^3} + 3\varepsilon u^2 v + 3\varepsilon^2 u v^2 + \varepsilon^3 v^3 - \cancel{u^3} \right) dx$$

$$= \lim_{\varepsilon \to 0} \int_0^L \left(3u^2 v + 3\varepsilon u v^2 + \varepsilon^2 v^3 \right) dx$$

$$= \int_0^L 3u^2 v\,dx$$

$$= \langle 3u^2, v \rangle \quad \forall v \in V$$

$$\Rightarrow \frac{\delta \mathcal{F}}{\delta u} = 3u^2$$

Hamiltonian PDEs [3]

Example ②: $\mathcal{F}[u] = \int_0^L \frac{1}{2} u_x^2 \, dx \Rightarrow \mathcal{F}[u+\varepsilon v] = \int_0^L \frac{(u_x+\varepsilon v_x)^2}{2} dx$

$$\Rightarrow \left\langle \frac{\delta \mathcal{F}}{\delta u}, v \right\rangle = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left(\int_0^L \frac{(u_x+\varepsilon v_x)^2}{2} dx - \int_0^L \frac{u_x^2}{2} dx \right)$$

$$= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \int_0^L \left(\frac{1}{2} \left(\cancel{u_x^2} + 2\varepsilon u_x v_x + \varepsilon^2 v_x^2 \right) - \cancel{\frac{1}{2} u_x^2} \right) dx$$

$$= \lim_{\varepsilon \to 0} \int_0^L \left(u_x v_x + \frac{1}{2} \varepsilon v_x^2 \right) dx$$

$$= \int_0^L u_x v_x = \cdots ? \qquad \left(\text{we need} \cdots : \int_0^L \cdots v \, dx \right)$$

Integration by parts: $\underbrace{u_x v \Big|_0^L}_{=0} - \int_0^L u_{xx} v \, dx = \langle -u_{xx}, v \rangle \quad \forall v \in V$

because $u_x(L) = u_x(0)$

$$\Rightarrow \frac{\delta \mathcal{F}}{\delta u} = -u_{xx}$$

Hamiltonian PDEs [4]

A general formula: $\mathcal{F}[u] = \int_0^L f(u, u_x, u_{xx}, u_{xxx}, \ldots)\, dx$

$$\Rightarrow \frac{\delta \mathcal{F}}{\delta u} = \frac{\partial f}{\partial u} - \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial u_x}\right) + \frac{\partial^2}{\partial x^2}\left(\frac{\partial f}{\partial u_{xx}}\right) \cdots = \sum_{k=0}^{\infty} (-1)^k \frac{\partial^k}{\partial x^k}\left(\frac{\partial f}{\partial u_{kx}}\right)$$

---

other cases: $\mathcal{F}[u,w] = \int_0^L \underbrace{u_x w}_{=f}\, dx \quad \Rightarrow \quad \frac{\delta \mathcal{F}}{\delta w} = u_x \,, \quad \frac{\delta \mathcal{F}}{\delta u} = -\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial u_x}\right) = -\frac{\partial}{\partial x} w = -w_x$

or: $\mathcal{F}[u] = \int_0^L \underbrace{u u_x^2}_{=f}\, dx$

$$\Rightarrow \frac{\partial f}{\partial u} = u_x^2 \,, \quad \frac{\partial f}{\partial u_x} = 2 u u_x \qquad \Rightarrow \frac{\delta \mathcal{F}}{\delta u} = \frac{\partial f}{\partial u} - \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial u_x}\right) = u_x^2 - \frac{\partial}{\partial x}(2 u u_x)$$

$$= u_x^2 - (2 u_x^2 + 2 u u_{xx}) = -u_x^2 - 2 u u_{xx}$$

Hamiltonian PDEs [5]

Hamiltonian PDE: $\boxed{\dfrac{\partial u}{\partial t} = \mathcal{J}\,\dfrac{\delta \mathcal{H}}{\delta u}}$

(functional $\mathcal{H}$)

operator $\mathcal{J}$ — skew-symmetric matrix; differential operator, e.g., $\mathcal{J} = \frac{\partial}{\partial x}$

a skew-symmetric operator with respect to innerproduct $\langle \cdot , \cdot \rangle$ $\Leftrightarrow \langle u, \mathcal{J} v\rangle = -\langle v, \mathcal{J} u\rangle \quad \forall u, v \in V$

skew-symmetric operator; check innerproduct (integral) and periodic BCs

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Example[1] Sine-Gordon equation $\boxed{q_{tt} = q_{xx} - \sin(q)}$ $\boxed{*}$

define $p = q_t$ and $\vec{u}(x,t) = (q(x,t), p(x,t))^T$

$$\mathcal{H}[q,p] = \int_0^L \left(\tfrac{1}{2}p^2 + \tfrac{1}{2}q_x^2 - \cos(q)\right)dx \quad \text{and} \quad \mathcal{J} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

$$\Rightarrow u_t = \mathcal{J}\,\frac{\delta\mathcal{H}}{\delta u} \Leftrightarrow \begin{pmatrix} q_t \\ p_t \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta \mathcal{H}}{\delta q} \\ \frac{\delta \mathcal{H}}{\delta p} \end{pmatrix} \Leftrightarrow \begin{cases} q_t = p \\ p_t = q_{xx} - \sin(q) \end{cases}$$

$$\Leftrightarrow \boxed{*}$$

Hamiltonian PDEs [6]

<u>Example</u>[2] advection equation $\boxed{u_t = u_x}$

$$\mathcal{H}[u] = \int_0^L \tfrac{1}{2} u^2 \, dx \quad \Rightarrow \quad \frac{\delta \mathcal{H}}{\delta u} = u \quad \text{and} \quad \mathcal{J} = \frac{\partial}{\partial x}$$

$$
\begin{aligned}
\Rightarrow \quad \frac{d}{dt}\mathcal{H}[u] &= \frac{d}{dt} \int_0^1 \tfrac{1}{2} u^2 \, dx \\
&= \int_0^L \tfrac{1}{2} \frac{d}{dt}(u^2) \, dx \\
&= \int_0^L u \, u_t \, dx \\
&\overset{\text{PDE}}{=} \int_0^L u \, u_x \, dx \\
&= \int_0^L \frac{\partial}{\partial x} \left(\tfrac{1}{2} u^2\right) dx \\
&= \tfrac{1}{2} u^2 \Big|_0^L = 0 \,, \quad \text{because } u(L) = u(0)
\end{aligned}
$$

Hamiltonian PDEs [7]

Similar calculation for sine-Gordon (Example 1):

$$\frac{d}{dt}\mathcal{H}[u] = \frac{d}{dt}\int_0^L \left(\tfrac{1}{2}p^2 + \tfrac{1}{2}q_x^2 - \cos(q)\right)dx$$

$\uparrow_{p,q}$

$$= \int_0^L \left(p\,p_t + q_x q_{xt} + \sin(q)\,q_t\right)dx$$

two PDEs (for q,p)

$$= \int_0^L \left(p\,(q_{xx} - \cancel{\sin(q)}) + q_x p_x + \cancel{\sin(q)}\,p\right)dx$$

$$= \int_0^L \left(p\,q_{xx} + q_x p_x\right)dx$$

integration by parts

$$= \underbrace{-\int_0^L p_x q_x\,dx + \int_0^L q_x p_x\,dx}_{=0} + \underbrace{p\,q_x\Big|_0^L}_{=0}$$

$$= 0$$

Hamiltonian PDEs [8]

Another conserved integral for the Sine-Gordon PDE:

"linear momentum" $M = \int_0^L p\, q_x\, dx$

check $\Rightarrow$ $\frac{d}{dt} M = \int_0^L (p\, q_x)_t\, dx$

$= \int_0^L (p_t\, q_x + p\, q_{xt})\, dx$

$= \int_0^L \left((q_{xx} - \sin(q))\, q_x + p\, p_x \right) dx$

$= \int_0^L \frac{\partial}{\partial x} \left[\frac{1}{2} q_x^2 + \cos(q) + \frac{1}{2} p^2 \right] dx$

$= \left(\frac{1}{2} q_x^2 + \cos(q) + \frac{1}{2} p^2 \right) \Big|_{x=0}^{x=L}$

$= 0$

$q_x(L) = q_x(0)$

$q(L) = q(0) \Rightarrow \cos(q(L)) = \cos(q(0))$

$p^2(L) = p^2(0)$

Hamiltonian PDEs [9]

In general: $\boxed{\frac{d}{dt}\mathcal{H}[u]} = \frac{d}{dt}\int_0^L f(u,u_x,\dots)\,dx = \int_0^L \frac{d}{dt} f(u,u_x,\dots)\,dx$

$$= \int_0^L \left[\frac{\partial f}{\partial u}u_t + \frac{\partial f}{\partial u_x}u_{xt} + \frac{\partial f}{\partial u_{xx}}u_{xxt} + \dots\right]dx$$

$$= \int_0^L \left[u_t \frac{\partial f}{\partial u} + \frac{\partial f}{\partial u_x}(u_t)_x + \frac{\partial f}{\partial u_{xx}}(u_t)_{xx} + \dots\right]dx$$

$u_t = \mathcal{J}\frac{\delta \mathcal{H}}{\delta u}$

$$= \int_0^L \left[u_t \frac{\partial f}{\partial u} + \frac{\partial f}{\partial u_x}\left(\mathcal{J}\frac{\delta\mathcal{H}}{\delta u}\right)_x + \frac{\partial f}{\partial u_{xx}}\left(\mathcal{J}\frac{\delta\mathcal{H}}{\delta u}\right)_{xx} + \dots\right]dx$$

$$\int_0^L \frac{\partial f}{\partial u_x}(u_t)_x\,dx = \underbrace{\frac{\partial f}{\partial u_x}u_t\Big|_0^L}_{=0} - \int_0^L \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial u_x}\right)u_t\,dx = -\int_0^L \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial u_x}\right)u_t\,dx$$

$$\dots = \int_0^L \left(u_t\frac{\partial f}{\partial u} - \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial u_x}\right)u_t + \dots\right)dx$$

$$= \left\langle u_t, \frac{\delta\mathcal{H}}{\delta u}\right\rangle = \left\langle \mathcal{J}\frac{\delta\mathcal{H}}{\delta u}, \frac{\delta\mathcal{H}}{\delta u}\right\rangle = \left\langle \frac{\delta\mathcal{H}}{\delta u}, \mathcal{J}\frac{\delta\mathcal{H}}{\delta u}\right\rangle = -\left\langle \mathcal{J}\frac{\delta\mathcal{H}}{\delta u}, \frac{\delta\mathcal{H}}{\delta u}\right\rangle$$

see earlier formula! PDE property innerproduct skew symmetry

$$\Rightarrow \boxed{\frac{d\mathcal{H}}{dt}=0}$$

Hamiltonian PDEs [10]

Hamiltonian spatial discretization

Ham. PDE $\xrightarrow{\text{method-of-lines}}$ system of Ham. ODEs

$\downarrow$ apply geometric/symplectic time-integration method (for example implicit midpoint)

grid: $x_i = i\Delta x$, $i = 0, 1, \dots, N$

$\Delta x = \frac{L}{N}$

periodic BCs: $u_N = u_0$ (etcetera)

define discrete inner product: $\langle u, v \rangle = \sum_{i=0}^{N-1} u_i v_i \Delta x$

scaling factor

$\left(u_i(t) \approx u(x_i, t) \right.$ "M.o.L." $\left. \right)$

Hamiltonian PDEs [11]

Remember Example ① $\mathcal{F}[u] = \int_0^L u^3\, dx$

then the (semi-) discrete Hamiltonian: $F[u] = \sum_{i=0}^{N-1} u_i^3 \Delta x$

$\left.\begin{matrix} \\ \\ \end{matrix}\right\}$ "$dx \leftrightarrow \Delta x$, $\int \leftrightarrow \sum$, $u \leftrightarrow u_i$"

variational derivative: $\left\langle \frac{\delta F}{\delta u}, v \right\rangle = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon}\left[F(u+\varepsilon v) - F(u) \right]$

$$= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon}\left(\sum_{i=0}^{N-1} \left((u_i + \varepsilon v_i)^3 - u_i^3 \right) \Delta x \right)$$

$$= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \sum_{i=0}^{N-1} \left(\cancel{u_i^3} + 3\varepsilon u_i^2 v_i + 3\varepsilon^2 u_i v_i^2 + \varepsilon^3 v_i^3 - \cancel{u_i^3} \right) \Delta x$$

$$= \lim_{\varepsilon \to 0} \sum_{i=0}^{N-1} \left(3u_i^2 v_i + 3\varepsilon u_i v_i^2 + \varepsilon^2 v_i^3 \right) \Delta x$$

$$= \sum_{i=0}^{N-1} 3u_i^2 v_i \,\Delta x = \langle u, v \rangle \quad \text{(discrete version)}$$

$$\Rightarrow \frac{\delta F}{\delta u} = 3u^2 \qquad \left(\text{or } \left(\frac{\delta F}{\delta u}\right)_i = 3u_i^2 \right)$$

componentwise (like u.^2 in Matlab)

Hamiltonian PDEs [12]

other example $\quad F(u) = \sum_{i=0}^{N-1} \frac{1}{2}\left(\frac{u_{i+1}-u_i}{\Delta x}\right)^2 \Delta x \quad \left(\sim \int_0^L \frac{1}{2} u_x^2\,dx = \mathcal{F}(u)\right)$

discrete $\qquad$ continuous

variational derivative: $\left\langle \frac{\delta F}{\delta u}, v\right\rangle = \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\sum_{i=0}^{N-1}\left(\frac{1}{2}\left(\frac{u_{i+1}+\varepsilon v_{i+1}-u_i-\varepsilon v_i}{\Delta x}\right)^2 - \frac{1}{2}\left(\frac{u_{i+1}-u_i}{\Delta x}\right)^2\right)\Delta x$

$$= \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\sum_{i=0}^{N-1}\frac{\Delta x}{2(\Delta x)^2}\left[\cancel{(u_{i+1}-u_i)^2} + 2\varepsilon(u_{i+1}-u_i)(v_{i+1}-v_i) + \varepsilon^2(v_{i+1}-v_i)^2 - \cancel{(u_{i+1}-u_i)^2}\right]$$

$$= \lim_{\varepsilon\to 0}\sum_{i=0}^{N-1}\frac{\Delta x}{2(\Delta x)^2}\left[2(u_{i+1}-u_i)(v_{i+1}-v_i) + \varepsilon(v_{i+1}-v_i)^2\right]$$

$$= \sum_{i=0}^{N-1}\frac{1}{(\Delta x)^2}(u_{i+1}-u_i)(v_{i+1}-v_i)\,\Delta x$$

This is NOT yet in the useful form of an inner product between ---- and v ! must find

Note that: "trick" $\quad \sum_{i=0}^{N-1} v_{i+1}(u_{i+1}-u_i)\Delta x = \sum_{i=0}^{N-1} v_i(u_i-u_{i-1})\Delta x$

why? → shift index by 1
→ make use of $v_N = v_0$, $u_N = u_0$
→ check that two terms cancel

$$= \sum_{i=0}^{N-1}\frac{1}{(\Delta x)^2}(u_i - u_{i-1} + u_i - u_{i+1})v_i\,\Delta x$$

$(u_{i+1}-u_i)(v_{i+1}-v_i) = \underbrace{(u_{i+1}-u_i)v_{i+1}}_{(--)} + (u_i-u_{i+1})v_i$

Hamiltonian PDEs [13]

$$= \sum_{i=0}^{N-1} - \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2} \cdot v_i \; \Delta x = \langle \cdots\cdots , v \rangle \quad \text{(discrete)}$$

$$\Rightarrow \left(\frac{\delta F}{\delta u}\right)_i = - \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2}, \quad i = 0, 1, \ldots, N-1$$

remember: $\frac{\delta \mathcal{F}}{\delta u} = -u_{xx}$

Summarized:
1) choose a quadrature (numerical integration) $H(u)$ to approximate the functional $\mathcal{H}(u)$
2) choose an approximation J (skew-symmetric) for operator $\mathcal{J}$

$$\Rightarrow \boxed{\dot{\vec{u}} = J \frac{\delta H}{\delta u}} \quad \text{(system of ODEs)}$$

3) apply a "geometric" or "symplectic" time-integration method (example: implicit midpoint, or ---- see Springer book on geometrical numerical integration by Hairer, Lubich, Wanner

Hamiltonian PDEs [14]

"symplectic structures"

example: the wave equation $\boxed{u_{tt} = u_{xx}}$

$$\mathcal{H} = \frac{1}{2}\int_0^L (u_x^2 + v^2)\,dx$$

$$\Updownarrow$$

$$\begin{cases} u_t = \dfrac{\delta \mathcal{H}}{\delta v} = v \\ v_t = -\dfrac{\delta \mathcal{H}}{\delta u} = u_{xx} \end{cases}$$

$$\Updownarrow$$

$$\begin{pmatrix} u \\ v \end{pmatrix}_t = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{\delta \mathcal{H}}{\delta u} \\ \frac{\delta \mathcal{H}}{\delta v} \end{pmatrix}$$

satisfies the symplectic form:

$$\frac{\partial}{\partial t}\underbrace{(du \wedge dv)}_{\underset{def}{=}\omega = du^T dv - dv^T du} = 0$$

(differentials)

*Hamiltonian PDEs [15]

extra : multi-symplectic $\leftrightarrow$ "symplectic in space and time"

$$\begin{cases} u_t = v \\ u_x = w \\ v_t - w_x = 0 \end{cases} \Longrightarrow \underbrace{\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{=M} \begin{pmatrix} u \\ v \\ w \end{pmatrix}_t + \underbrace{\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}}_{=K} \begin{pmatrix} u \\ v \\ w \end{pmatrix}_x = \begin{pmatrix} 0 \\ v \\ -w \end{pmatrix}$$

$$M\vec{z}_t + K\vec{z}_x = \nabla_{\vec{z}} S$$

$$\vec{z} = \begin{pmatrix} u \\ v \\ w \end{pmatrix}, \quad S = \tfrac{1}{2}(v^2 - w^2)$$

$$\frac{\partial}{\partial t}\underbrace{[du \wedge dv]}_{=\omega} + \frac{\partial}{\partial x}\underbrace{[du \wedge dw]}_{=\kappa} = 0$$

"conservation of symplecticity"