GEOMETRIC INTEGRATION IN CELESTIAL MECHANICS VIA THE CONTACT LENSES

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with

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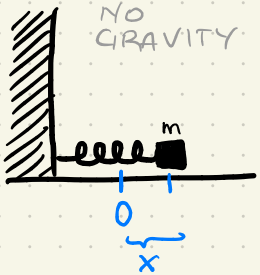
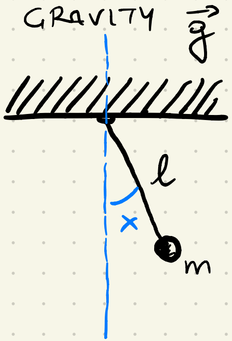
MATHEMATIC COLLOQUIUM – VU AMSTERDAM – 22.02.2023

CONSERVATIVE SYSTEMS : NEWTON, LAGRANGE & HAMILTON

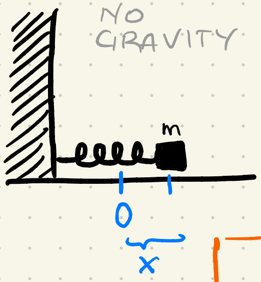


$$\begin{tikzcd}
 & L = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} k x^2 \arrow[dl, "EL"'] \arrow[dr] & \\
m \ddot{x} = -k x & & p = \frac{\partial L}{\partial \dot{x}} = m \dot{x} \arrow[dl] \\
 & H = \frac{1}{2m} p^2 + \frac{1}{2} k x^2 \arrow[ul, "HE"] &
\end{tikzcd}$$



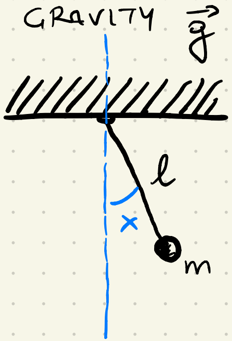
$$\begin{tikzcd}
 & L = \frac{1}{2} \dot{x}^2 + \frac{g}{\ell} \cos x \arrow[dl, "EL"'] \arrow[dr] & \\
\cancel{m} \ell \ddot{x} = - \cancel{m} g \sin x & & p = \frac{\partial L}{\partial \dot{x}} = \dot{x} \arrow[dl] \\
 & H = \frac{1}{2} p^2 - \frac{g}{\ell} \cos x \arrow[ul, "HE"] &
\end{tikzcd}$$

CONSERVATIVE SYSTEMS : NEWTON, LAGRANGE & HAMILTON



$$\begin{tikzcd} & L = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} k x^2 \arrow[ld, "EL"'] \arrow[dd, bend left, "p = \frac{\partial L}{\partial \dot{x}} = m \dot{x}"] \\ m \ddot{x} = -k x & \\ & H = \frac{1}{2m} p^2 + \frac{1}{2} k x^2 \arrow[lu, "HE"] \end{tikzcd}$$

H is constant along solutions to the equations of motion ⇝ can we guarantee this when performing numerics?



$$\begin{tikzcd} & L = \frac{1}{2} \dot{x}^2 + \frac{g}{\ell} \cos x \arrow[ld, "EL"'] \arrow[dd, bend left, "p = \frac{\partial L}{\partial \dot{x}} = \dot{x}"] \\ \cancel{m} \ell \ddot{x} = - \cancel{m} g \sin x & \\ & H = \frac{1}{2} p^2 - \frac{g}{\ell} \cos x \arrow[lu, "HE"] \end{tikzcd}$$

UNFORTUNATELY...

H is constant along solutions to the equations of motion ⤳ can we guarantee this when performing numerics!

$$H(q,p) = \frac{p^2}{2} + \frac{q^2}{2} \Rightarrow \begin{pmatrix}\dot q\\ \dot p\end{pmatrix} = \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}\begin{pmatrix}q\\ p\end{pmatrix}$$

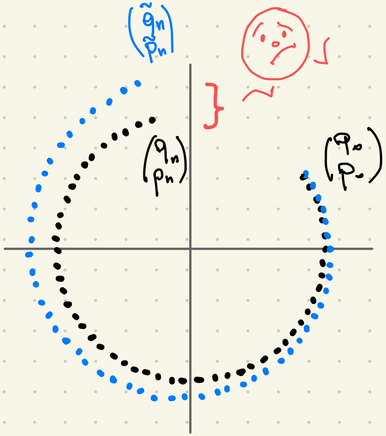
EXACT SOLUTION

$$\begin{pmatrix}q(t)\\ p(t)\end{pmatrix} = \begin{pmatrix}\cos t & \sin t\\ -\sin t & \cos t\end{pmatrix}\begin{pmatrix}q_0\\ p_0\end{pmatrix}$$

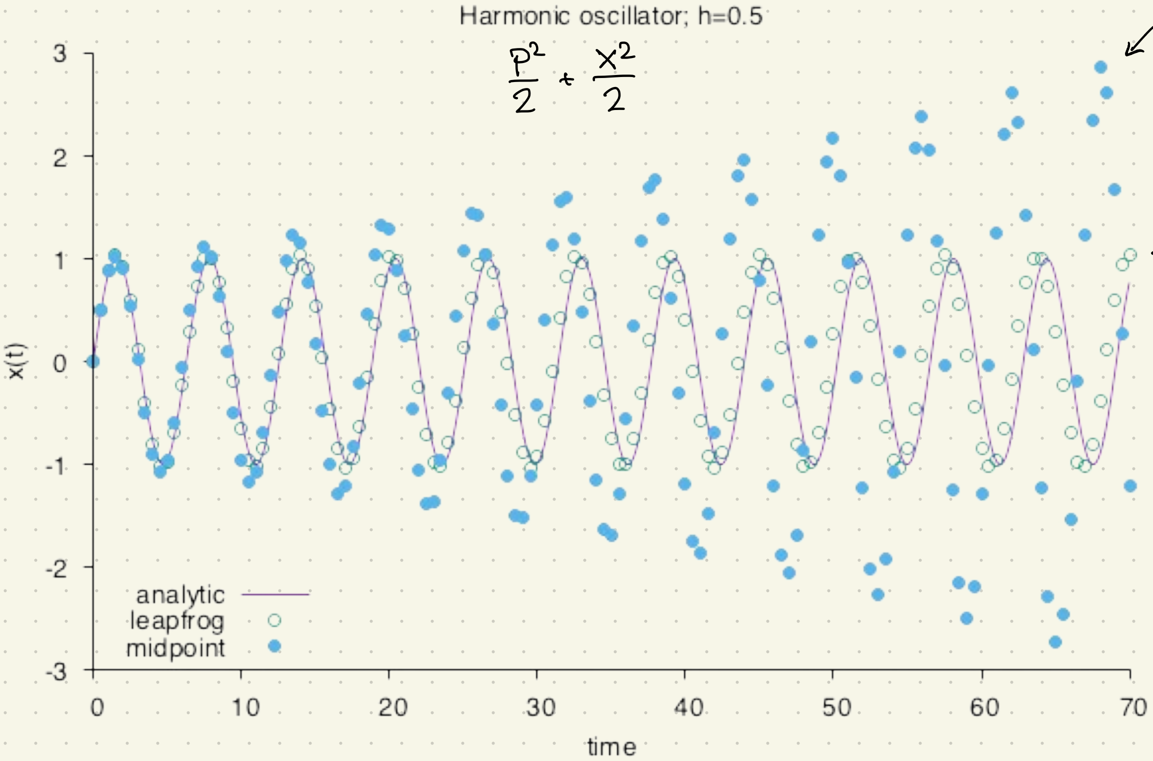
EULER METHOD (NUMERICAL, TIMESTEP $h=0.2$)

$$\begin{pmatrix}\tilde q_n\\ \tilde p_n\end{pmatrix} = \begin{pmatrix}1 & h\\ -h & 1\end{pmatrix}\begin{pmatrix}\tilde q_{n-1}\\ \tilde p_{n-1}\end{pmatrix}$$

$$\begin{pmatrix}q_n\\ p_n\end{pmatrix} := \begin{pmatrix}q(n\cdot h)\\ p(n\cdot h)\end{pmatrix}$$



HOWEVER

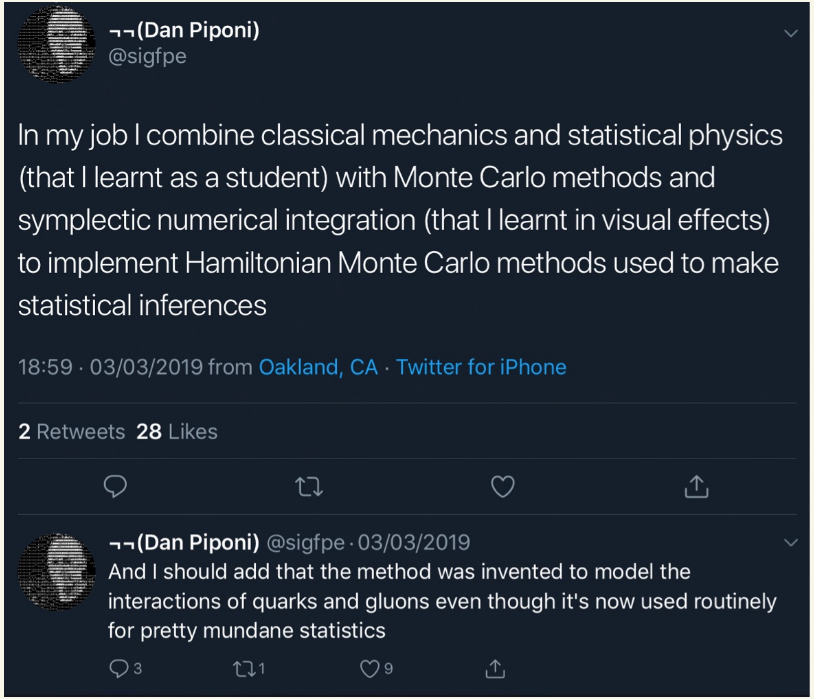


$$\frac{p^2}{2} + \frac{x^2}{2}$$

second order integretor

$\leftarrow$ 2^{nd} order symplectic integrator

NOT JUST THEORETICALLY INTERESTING...



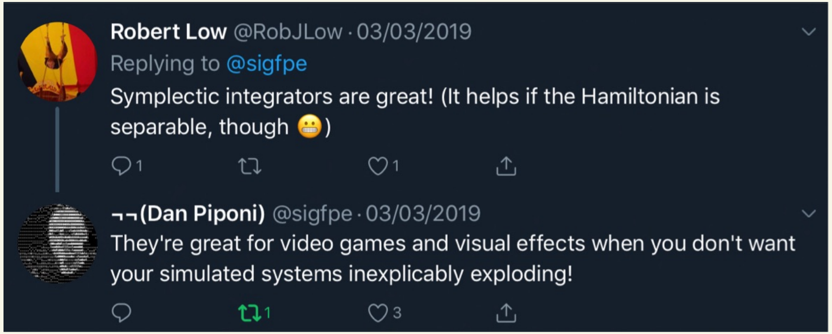
¬¬(Dan Piponi)
@sigfpe

In my job I combine classical mechanics and statistical physics (that I learnt as a student) with Monte Carlo methods and symplectic numerical integration (that I learnt in visual effects) to implement Hamiltonian Monte Carlo methods used to make statistical inferences

18:59 · 03/03/2019 from Oakland, CA · Twitter for iPhone

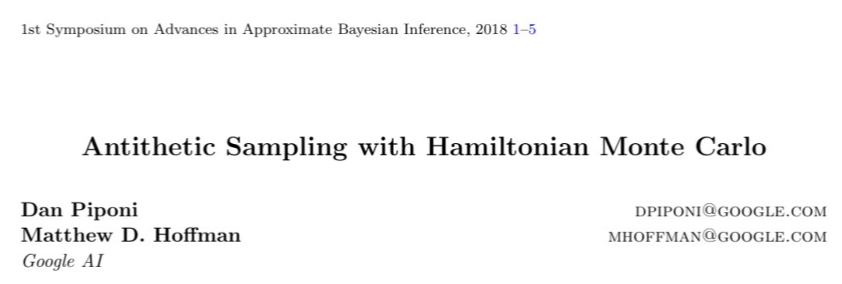
2 Retweets **28** Likes

¬¬(Dan Piponi) @sigfpe · 03/03/2019
And I should add that the method was invented to model the interactions of quarks and gluons even though it's now used routinely for pretty mundane statistics



Robert Low @RobJLow · 03/03/2019
Replying to @sigfpe
Symplectic integrators are great! (It helps if the Hamiltonian is separable, though 😬)

¬¬(Dan Piponi) @sigfpe · 03/03/2019
They're great for video games and visual effects when you don't want your simulated systems inexplicably exploding!



1st Symposium on Advances in Approximate Bayesian Inference, 2018 1–5

Antithetic Sampling with Hamiltonian Monte Carlo

Dan Piponi DPIPONI@GOOGLE.COM
Matthew D. Hoffman MHOFFMAN@GOOGLE.COM
Google AI

In principle, there is also great potential for applications

MANY INTERESTING NONCONSERVATIVE SYSTEMS

... are described by a slight modification of Newton's equations from the previous slide:

$$\ddot{x} = \underbrace{-\nabla V(x)}_{\text{NEWTON'S LAW AS SEEN BEFORE}} \underbrace{-\alpha(t)\dot{x}}_{\text{viscous damping with ratio } \alpha > 0} + \overbrace{f(t)}^{\text{external forcing } f(t)}$$

for example

Spin-Orbit model $\quad C\ddot{\theta} + \frac{dC}{dt}\dot{\theta} = N_Z(\theta, t)$ $\quad \left(\begin{array}{l} C \text{ moment of inertia} \\ \dot{\theta} \text{ angular velocity} \\ N_Z \text{ external torque} \end{array} \right)$

Families of perturbed kepler problems $\quad \ddot{x} + \frac{x}{|x|^3} = F(t, x, \dot{x})$

and more ...

MANY INTERESTING NONCONSERVATIVE SYSTEMS

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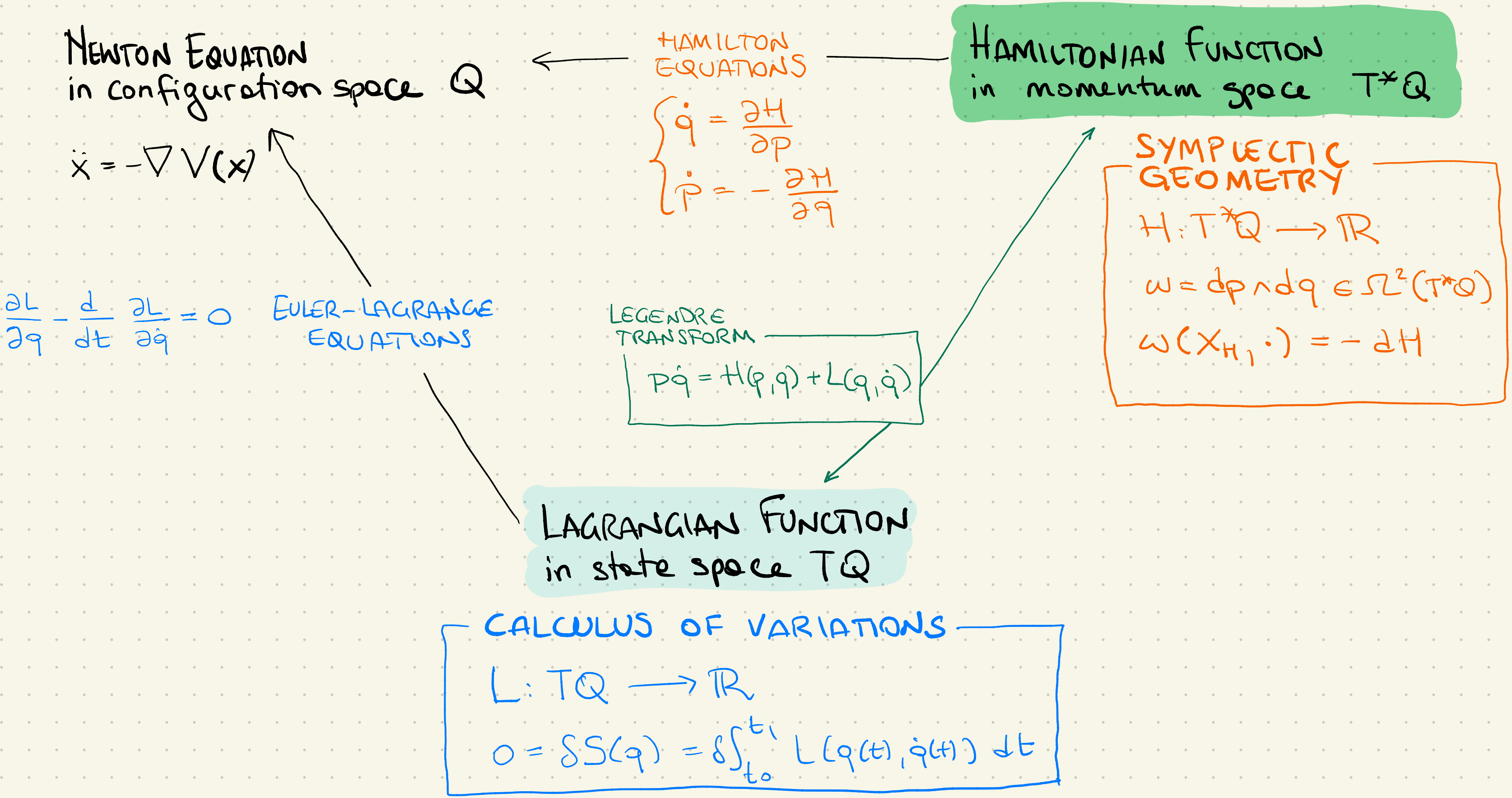
$\Longrightarrow$?

- Do we still have a geometric structure?
- Do we still have a variational formulation?
- Does it make any sense to find the corresponding geometric integrators?

OUTLINE

- CLASSICAL THEORY
  - A BRIEF RECAP OF (CONSERVATIVE) CLASSICAL MECHANICS
  - SYMPLECTIC INTEGRATORS 101
- CONTACT MECHANICS
  - CONTACT HAMILTONIAN MECHANICS IN A NUTSHELL
  - CONTACT LAGRANGIAN MECHANICS IN A NUTSHELL
- CONTACT INTEGRATION
  - CONTACT VARIATIONAL INTEGRATORS
  - CONTACT HAMILTONIAN INTEGRATORS (BRIEFLY)

NEWTON, LAGRANGE & HAMILTON: REPRISE



NEWTON EQUATION
in configuration space Q

$$\ddot{x} = -\nabla V(x)$$

HAMILTON EQUATIONS

$$\begin{cases} \dot{q} = \frac{\partial H}{\partial p} \\ \dot{p} = -\frac{\partial H}{\partial q} \end{cases}$$

HAMILTONIAN FUNCTION
in momentum space T^*Q

SYMPLECTIC GEOMETRY

$$H : T^*Q \longrightarrow \mathbb{R}$$

$$\omega = dp \wedge dq \in \Omega^2(T^*Q)$$

$$\omega(X_H, \cdot) = -dH$$

$$\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = 0$$

EULER-LAGRANGE EQUATIONS

LEGENDRE TRANSFORM

$$p\dot{q} = H(p,q) + L(q,\dot{q})$$

LAGRANGIAN FUNCTION
in state space TQ

CALCULUS OF VARIATIONS

$$L : TQ \longrightarrow \mathbb{R}$$

$$0 = \delta S(q) = \delta \int_{t_0}^{t_1} L(q(t), \dot{q}(t))\, dt$$

SYMPLECTIC GEOMETRY IN A NUTSHELL

(SYMPLECTIC FORM)

Smooth manifold M $\boxplus$ closed non-degenerate differential 2-form ω

$\Rightarrow$ morphism b/w $H : M \longrightarrow \mathbb{R}$ and $X_H : M \longrightarrow TM$

$$\omega(X_H, \bullet) = -dH$$

E.g. $M = T^*\mathbb{R}$, $\omega = dp \wedge dq$ $\Rightarrow$ $X_H = \left(\frac{\partial H}{\partial p}, -\frac{\partial H}{\partial q}\right)$

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Smooth manifold M $\boxplus$ closed non-degenerate differential 2-form ω

$\Longrightarrow$ isomorphism bw $H: M \longrightarrow \mathbb{R}$ and $X_H : M \longrightarrow TM$

$$\omega(X_H, \cdot) = -dH$$

$\Longrightarrow$

- dim $M = 2n$ and locally $\omega = dp \wedge dq$
- H constant along its flow : $dH(X_H) = -\omega(X_H, X_H) = 0$
- ω is invariant along the flow : $\mathcal{L}_{X_H}\omega = d(i_{X_H}\omega) + i_{X_H}(d\omega) = 0$

SYMPLECTIC GEOMETRY IN A NUTSHELL

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$\varphi : M \longrightarrow M$ **SYMPLECTIC MAP** if $\varphi^* \omega = \omega$ $\Rightarrow$ e^{tX_H} is symplectic!

SYMPLECTIC INTEGRATORS

A SYMPLECTIC INTEGRATOR IS A NUMERICAL SCHEME WHOSE DISCRETE TIME STEPS ARE SYMPLECTIC MAPS

SYMPLECTIC INTEGRATORS

A SYMPLECTIC INTEGRATOR IS A NUMERICAL SCHEME WHOSE DISCRETE TIME STEPS ARE SYMPLECTIC MAPS

VARIATIONAL

Discretization of the Lagrangian leads to Discrete action whose critical curves are the discrete time steps

HAMILTONIAN

Discretization of Hamilton's equations such that the time steps are Hamiltonian flows

Symplectic Integrators

A SYMPLECTIC INTEGRATOR IS A NUMERICAL SCHEME WHOSE DISCRETE TIME STEPS ARE SYMPLECTIC MAPS

VARIATIONAL

Discretization of the Lagrangian leads to Discrete action whose critical curves are the discrete time steps

MARSDEN, WEST - ACTA NUMERICA - 2001

e.g. $$L_{disc}(q_k, q_{k+1}) \approx L\left(q_k, \frac{q_{k+1}-q_k}{h}\right)$$

$$\rightsquigarrow S_{disc}(x) = \sum_{j=1}^{n} h \, L_{disc}(x_{j-1}, x_j)$$

⇝ DISCRETE EULER-LAGRANGE EQUATIONS

$$D_1 L_{disc}(x_j, x_{j+1}) + D_2 L_{disc}(x_{j-1}, x_j) = 0$$

⊕ DISCRETE LEGENDRE TRANSFORMS

$$p_j^{+} = -D_1 L_{disc}(x_j, x_{j+1})$$

$$p_j^{-} = D_2 L_{disc}(x_{j-1}, x_j)$$

LEAPFROG (OR STÖRMER-VERLET) INTEGRATOR

$$L_{disc} = \frac{1}{2} L\left(x_j, \frac{x_{j+1}-x_j}{h}\right) + \frac{1}{2} L\left(x_{j+1}, \frac{x_{j+1}-x_j}{h}\right)$$

$$\ddot{q} = -\nabla V(q) \rightsquigarrow L(q,\dot{q}) = \frac{1}{2}|\dot{q}|^2 - V(q)$$

$$\Downarrow$$

$$L_{disc}(x_j, x_{j+1}) = \frac{1}{2}\left|\frac{x_{j+1}-x_j}{h}\right|^2 - \frac{1}{2}\left(V(x_j) + V(x_{j+1})\right)$$

$\Rightarrow$ discrete Euler-Lagrange equation $\dfrac{x_{j+1} - 2x_j + x_{j-1}}{h} + V'(x_j) = 0$

$$\Rightarrow \begin{cases} x_{j+1} = x_j + h p_j - \frac{h^2}{2} V'(x_j) \\ p_{j+1} = p_j - \frac{h}{2}\left(V'(x_j) + V'(x_{j+1})\right) \end{cases}$$

LEAPFROG INTEGRATOR FROM MOTIVATION SLIDE

MARSDEN, WEST - ACTA NUMERICA - 2001

LEAPFROG (OR STÖRMER-VERLET) INTEGRATOR

$$L_{disc} = \frac{1}{2} L\left(x_j, \frac{x_{j+1}-x_j}{h}\right) + \frac{1}{2} L\left(x_{j+1}, \frac{x_{j+1}-x_j}{h}\right)$$

$$\ddot{q} = -\nabla V(q) \rightsquigarrow L(q,\dot{q}) = \frac{1}{2}|\dot{q}|^2 - V(q)$$

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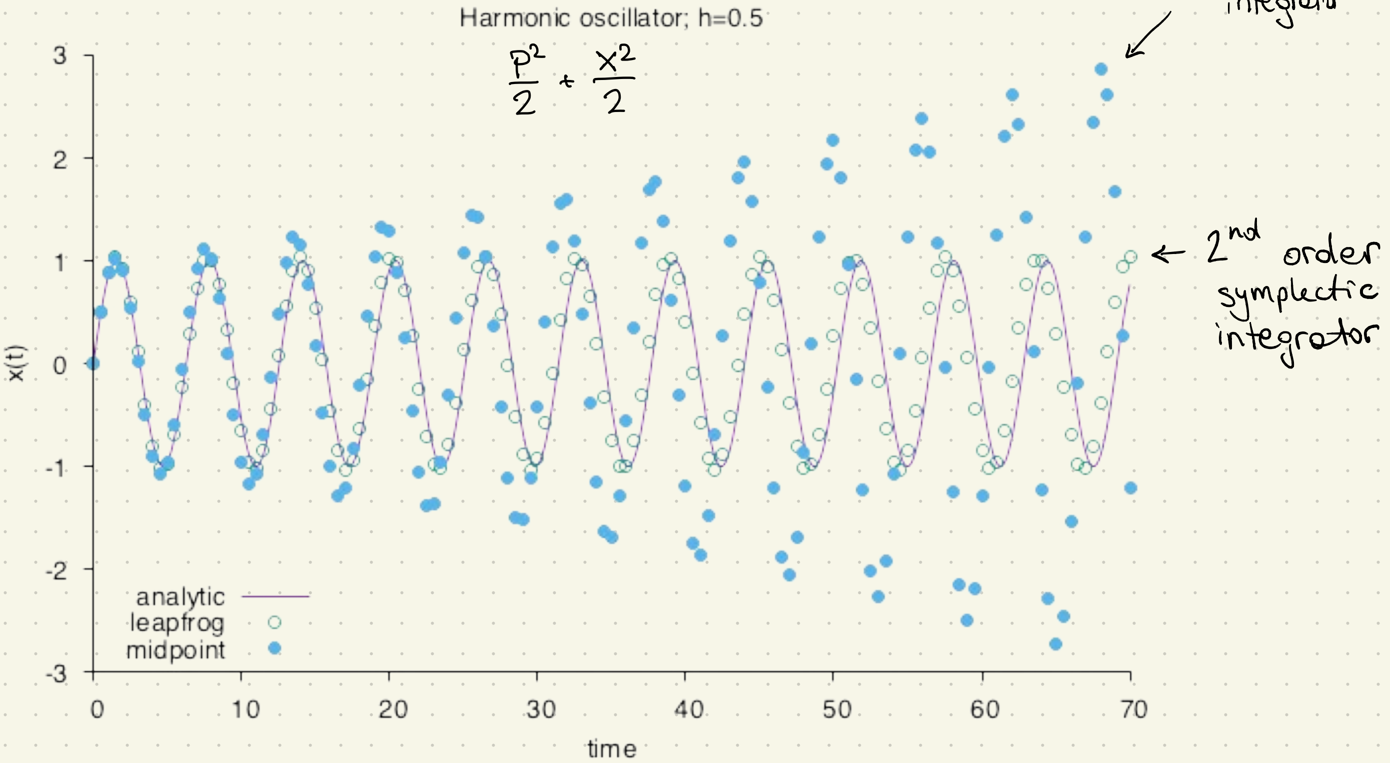
$x_{j+1} = x_j + h V'(x_j)$ Euler (1st ord)

$x_{j+1} = x_j + h V'(x_j + \frac{1}{2} h V'(x_j))$ Midpoint (2nd ord)

MARSDEN, WEST - ACTA NUMERICA - 2001

HOWEVER



Harmonic oscillator; h=0.5
$\frac{p^2}{2} + \frac{x^2}{2}$
x(t)
3
2
1
0
-1
-2
-3
time
0
10
20
30
40
50
60
70
analytic
leapfrog
midpoint
second order integrator
2^{nd} order symplectic integrator

HOW ABOUT NON CONSERVATIVE MECHANICS?

$$\underbrace{\ddot{q} = -V'(q)}_{\text{NEWTON'S LAW AS SEEN BEFORE}} \underbrace{- \alpha \dot{q}}_{\text{viscous damping with ratio } \alpha > 0} + \overbrace{f(t)}^{\text{external forcing } f(t)}$$

CONTACT HAMILTONIAN SYSTEMS TO THE RESCUE

Forget about time dependence (for now).

SYMPLECTIC GEOMETRY (HAMILTONIAN SYSTEMS) : M^{2n} with special 2-form ω (inducing volume ω^n)

CONTACT GEOMETRY : M^{2n+1} with special 1-form η (inducing volume $\eta \wedge (d\eta)^n$)

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maximally non-integrable distribution of hyperplanes (contact structure)

Contact Hamiltonian Systems to the Rescue

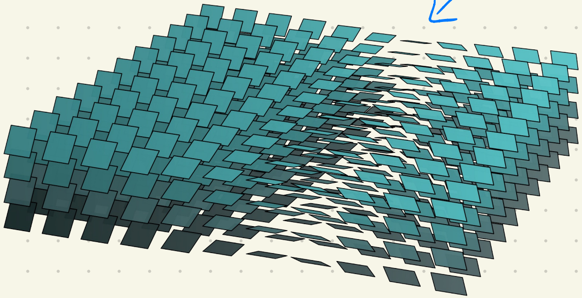
Forget about time dependence (for now).

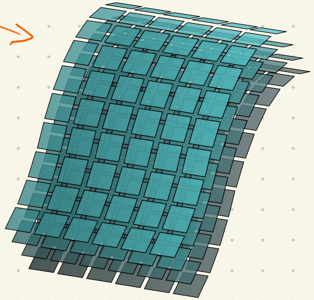
SYMPLECTIC GEOMETRY (HAMILTONIAN SYSTEMS) : M^{2n} with special 2-form ω (inducing volume ω^n)

CONTACT GEOMETRY : M^{2n+1} with $\underbrace{\text{special 1-form } \eta}_{\ker(\eta) \subset TM}$ (inducing volume $\eta \wedge (d\eta)^n$)

LOOKS LIKE

DOES **NOT** LOOK LIKE





Source: German Wikipedia

CONTACT HAMILTONIAN VECTOR FIELDS

<u>Claim</u>: the extra space & a contact form is what we need

Say $M = \mathbb{R}^{2n+1} \ni (q, p, s)$ and $\eta = ds - p\,dq$

⇒ morphism b/w $H : M \longrightarrow \mathbb{R}$ and $X_H : M \rightarrow TM$ via

$$\mathcal{L}_{X_H} \eta = -H \quad \text{and} \quad \mathcal{L}_{X_H} d\eta = dH + \rho_H \eta$$

CONTACT HAMILTONIAN VECTOR FIELDS

Claim: the extra space & a contact form is what we need

Say $M = \mathbb{R}^{2n+1} \ni (q, p, s)$ and $\eta = ds - p\,dq$

$\Rightarrow$ morphism bw $H : M \longrightarrow \mathbb{R}$ and $X_H : M \to TM$ via

$$\iota_{X_H} \eta = -H \quad \text{and} \quad \underbrace{\iota_{X_H} d\eta = dH + \boxed{\rho_H}\, \eta}$$

$$-\mathcal{L}_R H = -R(H)$$

where

$$\begin{cases} \eta(R) = 1 \\ d\eta(R) = 0 \end{cases}$$

Reeb vector field

$\rightsquigarrow R = \dfrac{\partial}{\partial s}$

$$\mathcal{L}_{X_H} \eta = \rho_H \eta$$

$\Rightarrow \ker(\eta)$ is preserved

CONTACT HAMILTONIAN VECTOR FIELDS

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$$\eta(X_H) = -H \quad \text{and} \quad \mathcal{L}_{X_H}\eta = \rho_H\,\eta \longleftarrow \text{ker}(\eta) \text{ is preserved}$$

$\varphi : M \longrightarrow M$ **CONTACT MAP** if $\varphi^*\eta = f_\varphi\,\eta$ for some $f_\varphi \neq 0$

CONTACT HAMILTONIAN VECTOR FIELDS

Say $M = \mathbb{R}^{2n+1} \ni (q, p, s)$ and $\eta = ds - p\,dq$

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$$\iota_{X_H} \eta = -H \quad \text{and} \quad \mathcal{L}_{X_H} \eta = \rho_H \eta$$

$\Rightarrow$ Equations of motion

$$\begin{cases} \dot{q} = \dfrac{\partial H}{\partial p} \\[2ex] \dot{p} = -\dfrac{\partial H}{\partial q} - p \dfrac{\partial H}{\partial s} \\[2ex] \dot{s} = p \dfrac{\partial H}{\partial p} - H \end{cases}$$

CONTACT HAMILTONIAN VECTOR FIELDS

Claim: the extra space is what we need

Say $M = \mathbb{R}^{2n+1} \ni (q, p, s)$ and $\eta = ds - p\,dq$

⇒ We can setup an isomorphism bw $H : M \longrightarrow \mathbb{R}$ and $X_H : M \to TM$ via

$$\iota_{X_H}\eta = -H \quad \text{and} \quad \mathcal{L}_{X_H}\eta = \rho_H\,\eta$$

⇒ Equations of motion

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E.g. $H = \frac{1}{2}p^2 + \frac{k}{2}q^2 + \alpha S$

$$\rightsquigarrow \begin{cases} \dot{q} = p \\ \dot{p} = -kq - \alpha p \\ \dot{S} = \frac{1}{2}p^2 - \frac{k}{2}q^2 - \alpha S \end{cases} \qquad \left.\begin{matrix} \\ \\ \end{matrix}\right\} \ddot{q} = -kq - \alpha\dot{q}$$

$$= p\dot{q} - H$$

CONTACT HAMILTONIAN VECTOR FIELDS

⊛ De Leon, Valcázar - JMP - 2019

Say $M = \mathbb{R}^{2n+1} \ni (q, p, s)$ and $\eta = ds - p\,dq$

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⇒ Equations of motion

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⊛ ⇝ • $\mathcal{L}_{X_H} H = \rho_H H = -\dfrac{\partial H}{\partial s} H$ ⇗ Energy not conserved unless $H = 0$ or $\dfrac{\partial H}{\partial s} = 0$

• $\mathcal{L}_{X_H}(\eta \wedge (d\eta)^n) = (n+1)\rho_H\, \eta \wedge (d\eta)^n$

⇓

volume preserved only if $\dfrac{\partial H}{\partial s} = 0$

yet,

$$\boxed{\Omega = H^{-(n+1)}\, \eta \wedge (d\eta)^n \quad \text{invariant}}$$

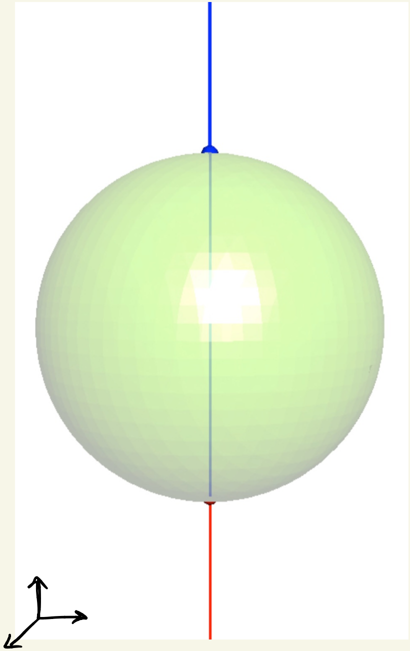
SOME EXAMPLES OF CONTACT HAMILTONIAN SYSTEMS

RAYLEIGH DISSIPATION	$\frac{\lvert p\rvert^2}{2} + V(q,t) + f(t)s$	
THERMODYNAMICS	$\left(\frac{e^{-\beta h(p,q)}}{Z} f(s)\right)^{-1/2}$	from 10.1103/PhysRevE.93.022139
COSMOLOGY	$\frac{\lvert p\rvert^2}{2} + V(q) + \gamma s^2$	from SLOAN-PhysRevD-2021
GENERIC	$\dot{x} = L\nabla_x E + M\nabla_x S$	from 10.1103/PhysRevE.56.6620
GRADIENT SYSTEMS	$\dot{x} = X(x)$ (via $\tilde{H}(x,p) = p \cdot X(x)$ $\oplus$ projection) from 10.3390/math9161960	

INTERESTING DYNAMICS OF COSMOLOGY DUMMY MODEL

$$H(q,p,s) = \frac{p^2}{2} + \gamma \frac{s^2}{2} + \frac{q^2}{2} - R$$

"cosmological contact oscillator"



Invariant subspaces:

- $H=0$ (green ellipsoid)
- $\{(0,0,s) \mid s \in \mathbb{R}\}$
- 2 fixed pts: attractive north pole & repelling south pole

  & ∞-many heteroclinic trajectories connecting them

DO WE ALSO HAVE A VARIATIONAL PRINCIPLE FOR THESE SYSTEMS?

HERGLOTZ VARIATIONAL PRINCIPLE

DEFN⊛ Let $L : \mathbb{R}_t \times TQ_{q,\dot{q}} \times \mathbb{R} \longrightarrow \mathbb{R}$. Given a curve $q : [0,T] \longrightarrow Q$, define $s : [0,T] \longrightarrow \mathbb{R}$ by an initial condition $s(0) = s_0$ and the differential equation $\dot{s}(t) = L(t, q(t), \dot{q}(t), s(t))$.

The curve q is a solution to HERGLOTZ' VARIATIONAL PRINCIPLE with initial condition s_0 if every variation of q that vanishes at the boundary of $[0,T]$ leaves the action $s(T)$ invariant.

⊛ First appearence is in Sophus Lie's notes, ~60 years before Herglotz paper

HERGLOTZ VARIATIONAL PRINCIPLE

DEFN* Let $L : \mathbb{R}_t \times TQ_{q,\dot{q}} \times \mathbb{R} \longrightarrow \mathbb{R}$. Given a curve $q : [0,T] \to Q$, define $s : [0,T] \to \mathbb{R}$ by an initial condition $s(0) = s_0$ and the differential equation $\dot{s}(t) = L(t, q(t), \dot{q}(t), s(t))$.

A curve q is a solution iff it satisfies the GENERALIZED EULER-LAGRANGE EQUATIONS

$$\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} + \frac{\partial L}{\partial s} \cdot \frac{\partial L}{\partial \dot{q}} = 0$$

Furthermore, the flow of the generalized Euler-Lagrange equation is a CONTACT TRANSFORMATION wrt $\eta = ds - p\,dq$

TWO PICTURES OF CONTACT MECHANICS

VARIATIONAL

ACTION: $\dot{s} = L(q, \dot{q}, s)$

GENERALISED E-L EQNS

$$\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} + \frac{\partial L}{\partial s}\frac{\partial L}{\partial \dot{q}} = 0$$

$\longleftrightarrow$ LEGENDRE TRANSFORM

HAMILTONIAN

$H = H(p, q, s) \oplus ds - p\,dq$

CONTACT HAM. EQNS

$$\begin{cases} \dot{q} = \dfrac{\partial H}{\partial p} \\ \dot{p} = -\dfrac{\partial H}{\partial \dot{q}} - p\dfrac{\partial H}{\partial s} \\ \dot{s} = p\dfrac{\partial H}{\partial p} - H \end{cases}$$

Exercise: check this for the damped oscillator

DISCRETE HERGLOTZ PRINCIPLE

HERGLOTZ: GIVEN L
CONSIDER THE ODE

$$\dot{s} = L(q,\dot{q},s)$$

$\Rightarrow$ $s(T)$ critical wrt variations of q

GIVEN A DISCRETE LAGRANGIAN L, CONSIDER

$$\frac{s_{j+1}-s_j}{h} = L(q_j, q_{j+1}, s_j) \quad \circledast$$

$j\in\{0,\dots,N\}$ $\oplus$ q_0, q_N and s_0 PRESCRIBED

The discrete curve defined by $\circledast$ is a solution of the DISCRETE HERGLOTZ VARIATIONAL PRINCIPLE iff S_N is critical under variations of $q=\{q_0,\dots,q_N\}$

DISCRETE GENERALIZED EULER-LAGRANGE EQNS

THM (VERMEEREN - BRAVETTI - S, 2019)

$\{x_0, \dots, x_N\}$ solves the discrete Herglotz variational principle iff it satisfies the GENERALISED DISCRETE EULER-LAGRANGE EQUATIONS

$$D_1 L(x_j, x_{j+1}, s_j) + D_2 L(x_{j-1}, x_j, s_{j-1})\big(1 + h\, D_3 L(x_j, x_{j+1}, s_j)\big) = 0$$

The corresponding map $(x_{j-1}, x_j, s_{j-1}) \mapsto (x_j, x_{j+1}, s_j)$ induces a map $(x_j, p_j, s_j) \longmapsto (x_{j+1}, p_{j+1}, s_{j+1})$ which is a contact map wrt $\eta = ds - p\,dx$

Contact Variational Integrators

Established the DISCRETE HERGLOTZ PRINCIPLE and its DISCRETE E-L EQUATIONS, the construction of contact integrators of any order proceed as in symplectic case.

⇒ what about the discrete momentum equations?

⤳ DISCRETE EULER-LAGRANGE EQUATIONS

$$D_1 L_{disc}(x_j, x_{j+1}) + D_2 L_{disc}(x_{j-1}, x_j) = 0$$

⊕ DISCRETE LEGENDRE TRANSFORMS

$$p_j = -D_1 L_{disc}(x_j, x_{j+1})$$

$$p_{j+1} = D_2 L_{disc}(x_j, x_{j+1})$$

CONTACT VARIATIONAL INTEGRATORS

THM (VERMEEREN - BRAVETTI - S, 2019)

The map $(x_{j-1}, x_j, s_{j-1}) \longmapsto (x_j, x_{j+1}, s_j)$ from the previous theorem induces a map $(x_{j-1}, p_{j-1}, s_{j-1}) \longmapsto (x_j, p_j, s_j)$ where

$$p_{j-1} = -\frac{h\, D_1 L(x_{j-1}, x_j, s_{j-1})}{1 + h\, D_3 L(x_{j-1}, x_j, s_{j-1})} \qquad p_j = h\, D_2 L(x_{j-1}, x_j, s_{j-1})$$

which is a contact map wrt $\eta = ds - p\,dx$

VERMEEREN, BRAVETTI, SERI - JPhys A - 2019

BRAVETTI, SERI, ZADRA - CEL. MECH DYN ASTRO - 2020 ← HIGHER ORDER

SIMOES, DE DIEGO, VALCAZAR, DE LEON - J NONLIN SCI - 2021 ← ALTERNATIVE PROOF

THE DAMPED OSCILLATOR

$$H = \frac{p^2}{2} + V(q) + \alpha S \xrightarrow{LT} L = \frac{\dot{q}^2}{2} - V(q) - \alpha S$$

DISCRETE
LAGRANGIAN
⊕
E-L EQNS

$$L(q_j, q_{j+1}, s_j, s_{j+1}) = \frac{1}{2}\left(\frac{q_{j+1} - q_j}{h}\right)^2 - \frac{V(q_j) + V(q_{j+1})}{2} - \alpha \frac{s_j + s_{j+1}}{2}$$

$$\frac{q_{j+1} - 2q_j + q_{j-1}}{h^2} = -V(q_j) - \alpha\left(\frac{q_j - q_{j-1}}{h} - \frac{h}{2} V'(q_j)\right)$$

CONTACT
LEAPFROG
INTEGRATOR →

$$\begin{cases} q_j = q_{j-1} + h\left(1 - \frac{h}{2}\alpha\right) p_{j-1} - \frac{h^2}{2} V'(q_{j-1}) \\ p_j = \dfrac{\left(1 - \frac{h}{2}\alpha\right) p_{j-1} - \frac{h}{2}\left(V'(q_j) + V'(q_{j-1})\right)}{1 + \frac{h}{2}\alpha} \end{cases}$$

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CONTACT
LEAPFROG
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$$\begin{cases} x_{j+1} = x_j + h p_j - \frac{h^2}{2} V'(x_j) \\ p_{j+1} = p_j - \frac{h}{2}\left(V'(x_j) + V'(x_{j+1})\right) \end{cases}$$

LEAPFROG
INTEGRATOR

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CONTACT
LEAPFROG
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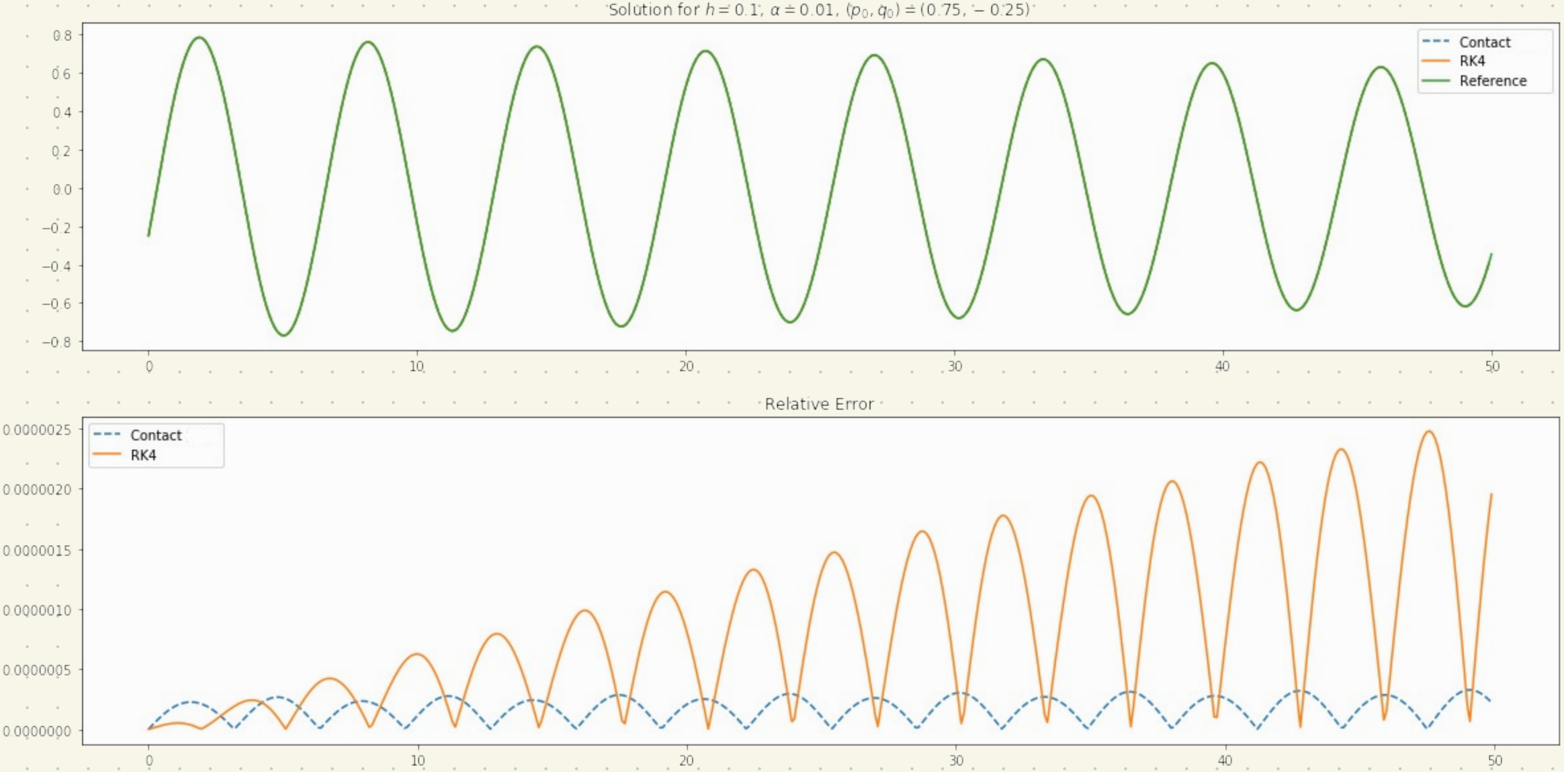
$$\Big\downarrow \; \alpha \to 0$$

✓

$$\begin{cases} x_{j+1} = x_j + h\,p_j - \frac{h^2}{2}V'(x_j) \\ p_{j+1} = p_j - \frac{h}{2}\left(V'(x_j) + V'(x_{j+1})\right) \end{cases}$$

LEAPFROG
INTEGRATOR

HOW DOES IT PERFORM?



WHAT ABOUT THE CONTACT HAMILTONIAN VERSION?

ASSUMPTION: $H(p,q,s) = \sum_{i=1}^{k} \varphi_i(q,p,s)$

Define

$$S_2(h) = e^{\frac{h}{2}X_{\varphi_k}} \cdots e^{\frac{h}{2}X_{\varphi_2}} e^{hX_{\varphi_1}} e^{\frac{h}{2}X_{\varphi_2}} \cdots e^{\frac{h}{2}X_{\varphi_k}}$$

THM (BRAVETTI, S, VERMEEREN, ZADRA 2020)

The map $x_k \mapsto x_{k+1} = S_2(h)x_k$ is a contact map wrt $ds-pdq$ and defines a second order numerical integrator, i.e. $\|e^{hX_H}x_k - S_2(h)x_k\| = O(h^3)$

here $x_k := (q_k, p_k, s_k)$

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here $x_k := (q_k, p_k, S_k)$

Can be explicitly computed! See Bravetti, S, Vermeeren, Zadra 2020 or arxiv:2210,11155

WHAT ABOUT HIGHER ORDERS?

YOSHIDA (1990)

$\exists\, m \in \mathbb{Z}$ and $\{w_j\}_{j=0}^{m} \subset \mathbb{R}$ such that

$$S^{(m)}(h) = S_2(w_m h)\, S_2(w_{m-1} h) \cdots S_2(w_0 h) \cdots S_2(w_{m-1} h)\, S_2(w_m h)$$

is an integrator of order 2ℓ

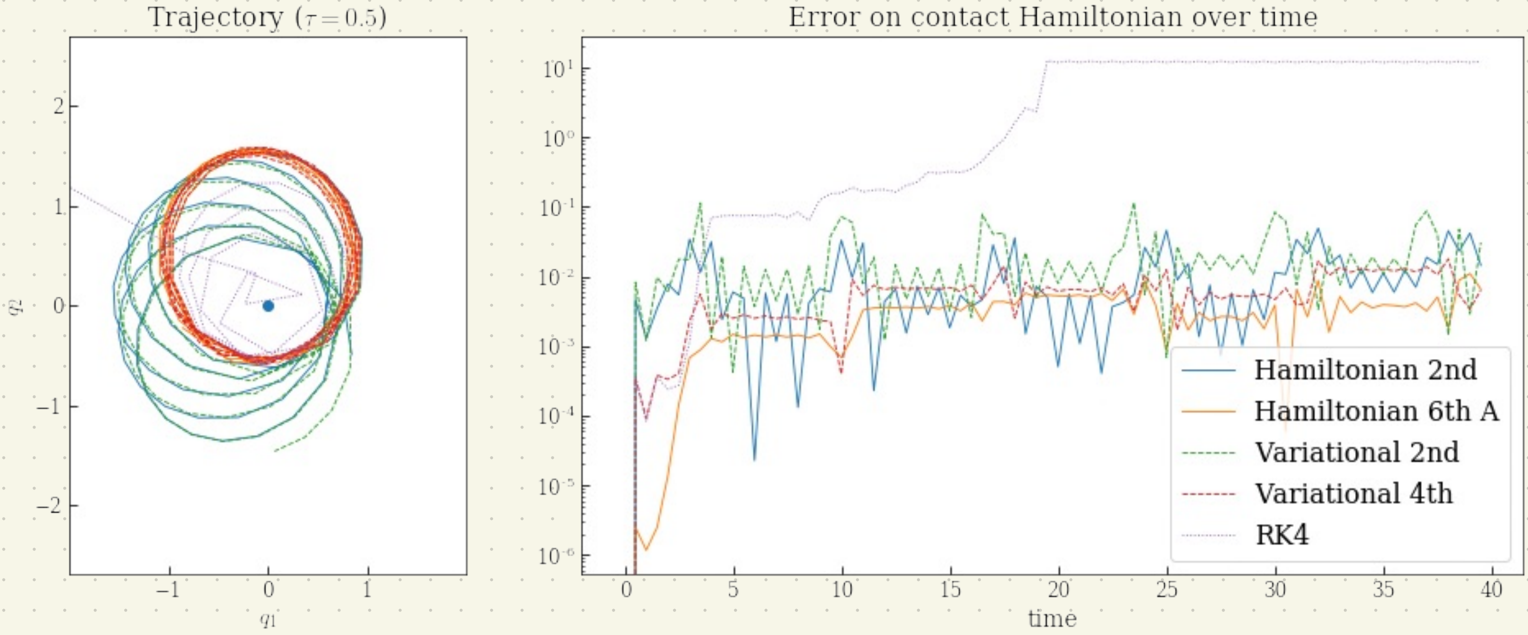
LEMMA (VBSZ 2020)

If S_2 is a contact map, also $S^{(m)}$ is a contact map

Remark For any fixed ℓ, neither m and $\{w_j\}$ are unique

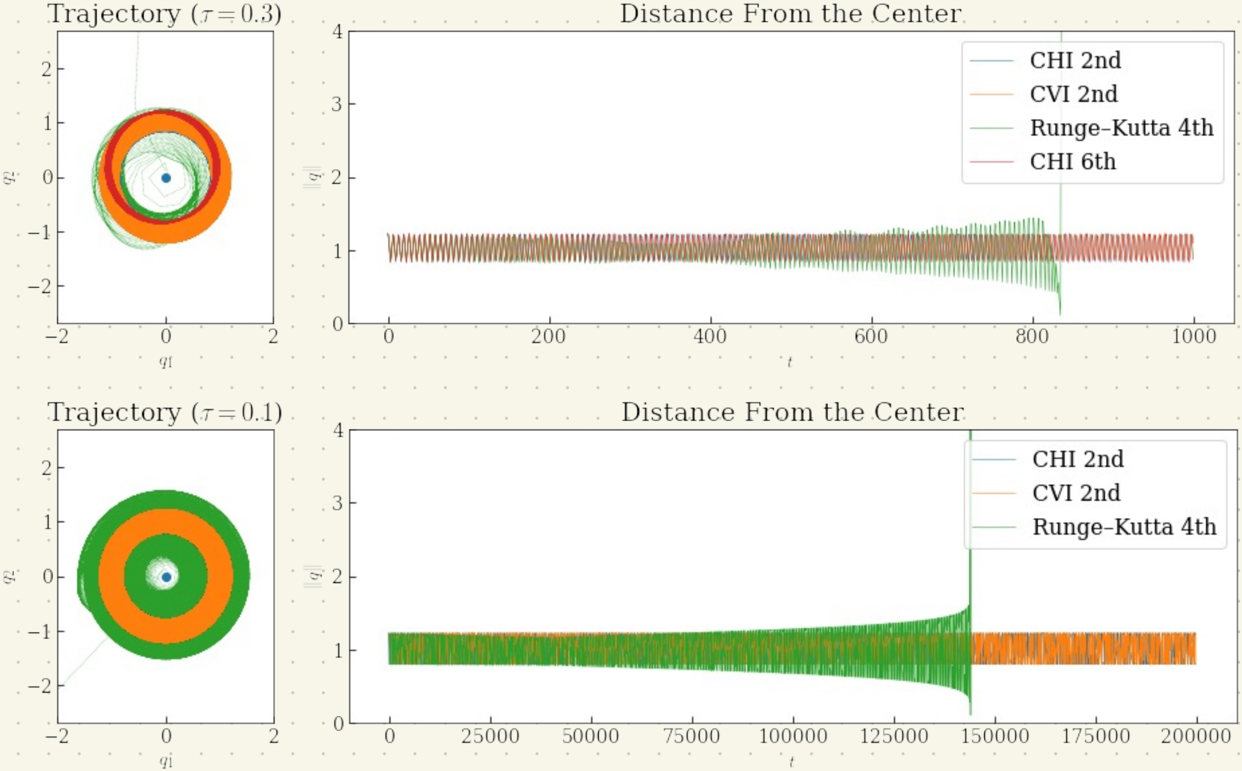
HOW DO THESE PERFORM?

PERTURBED KEPLER $H = \frac{|p|^2}{2} + \alpha \sin(\pi t) s + \frac{\gamma}{|q|}$



HOW DO THESE PERFORM?

PERTURBED KEPLER $H = \frac{|p|^2}{2} + \alpha \sin(\pi t) s + \frac{\gamma}{|q|}$



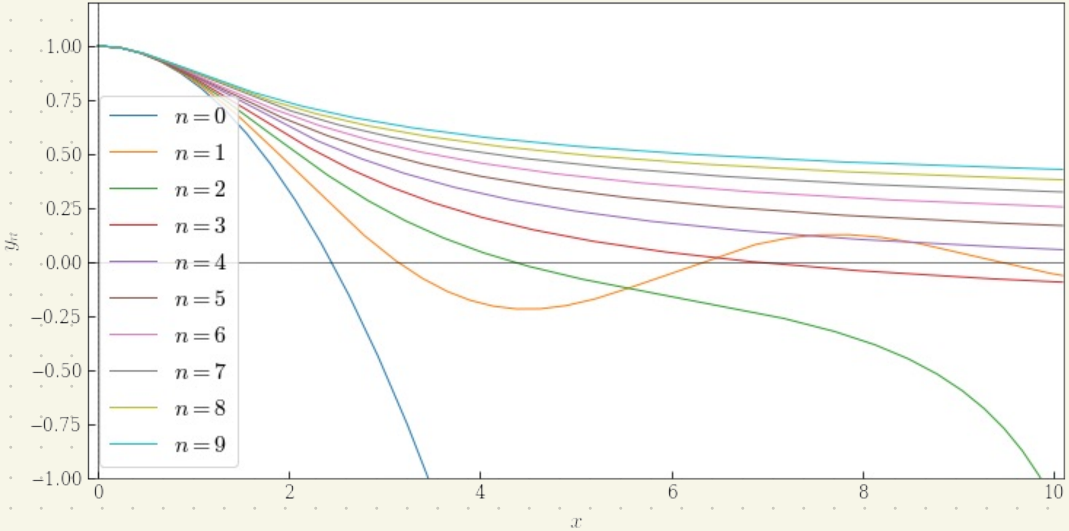
HOW DO THESE PERFORM?

LANE-EMDEN EQUATION

$$y''(x) + \frac{2}{x}y'(x) + y^n(x) = 0, \quad y(0) = 1, \; y'(0) = 0$$

$$y \mapsto q, \quad y' \mapsto p, \quad x \longmapsto t \quad \Rightarrow \quad \mathcal{H} = \frac{p^2}{2} + \frac{q^{n+1}}{n+1} + \frac{2}{t}S$$

Contact Hamiltonian, singular at 0

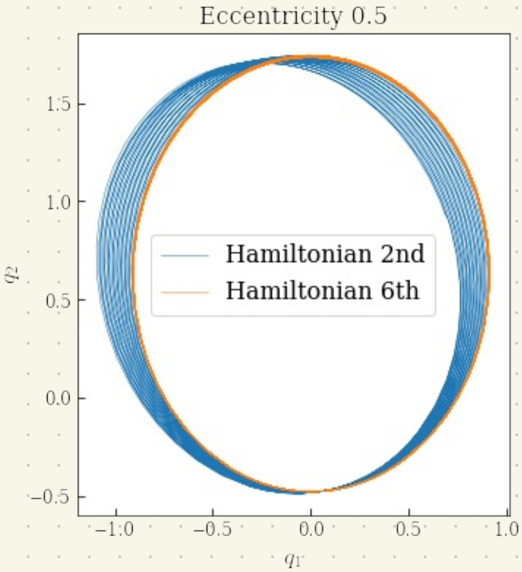


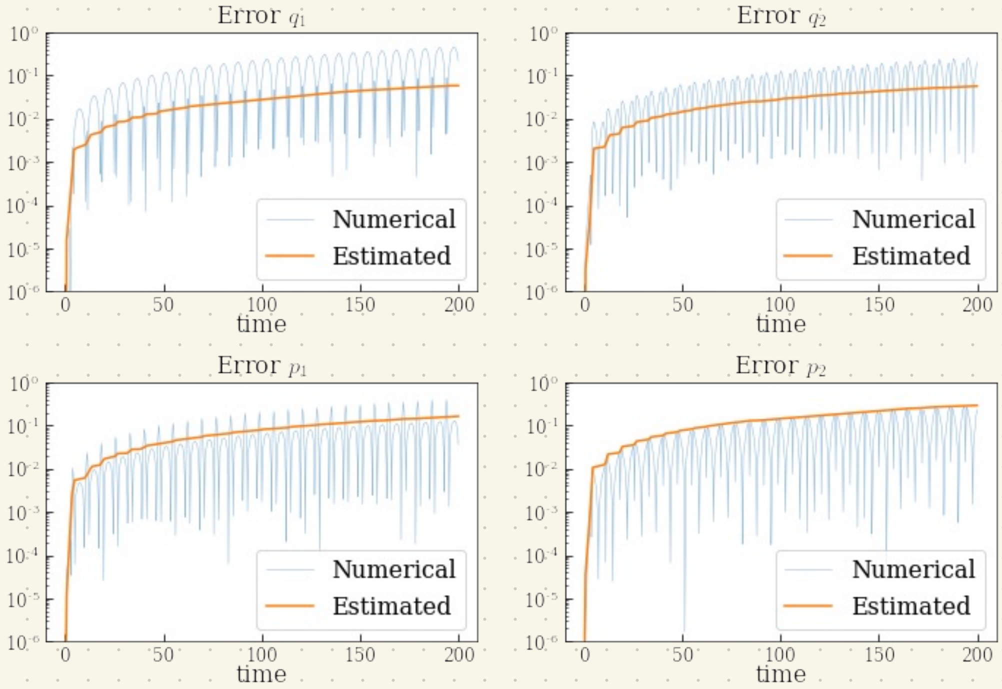
Numerically integrated solutions with $h=0.01$
$S(0)=0$

Error bounded above by 10^{-3} !
(and better in fact $\sim 10^{-5}$)

SOME EXAMPLES (WHERE THE ROLE OF h IS CLARIFIED)

PERTURBED KEPLER $H = \frac{|p|^2}{2} + \alpha \sin(\pi t) s + \frac{\gamma}{|q|}$

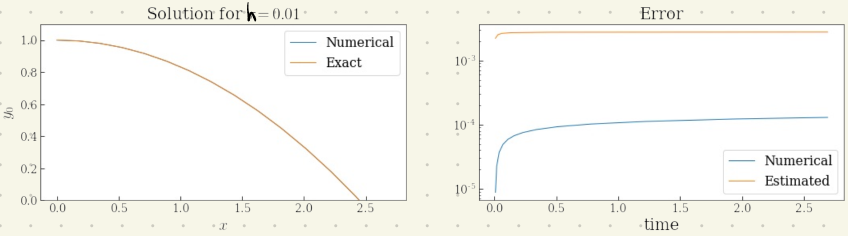




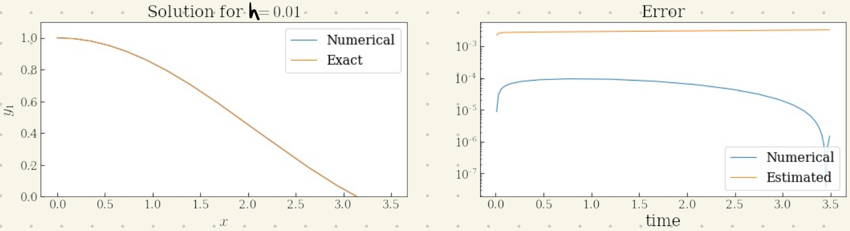
h=0.05 not enough to control $O(h^4)$

SOME EXAMPLES (WHERE THE ROLE OF h IS CLARIFIED)

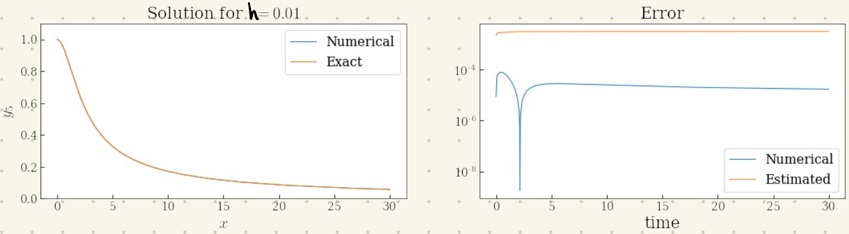
LANE-EMDEN CRUDE ESTIMATES compared to cases with explicit solutions



$n=0$



$n=1$

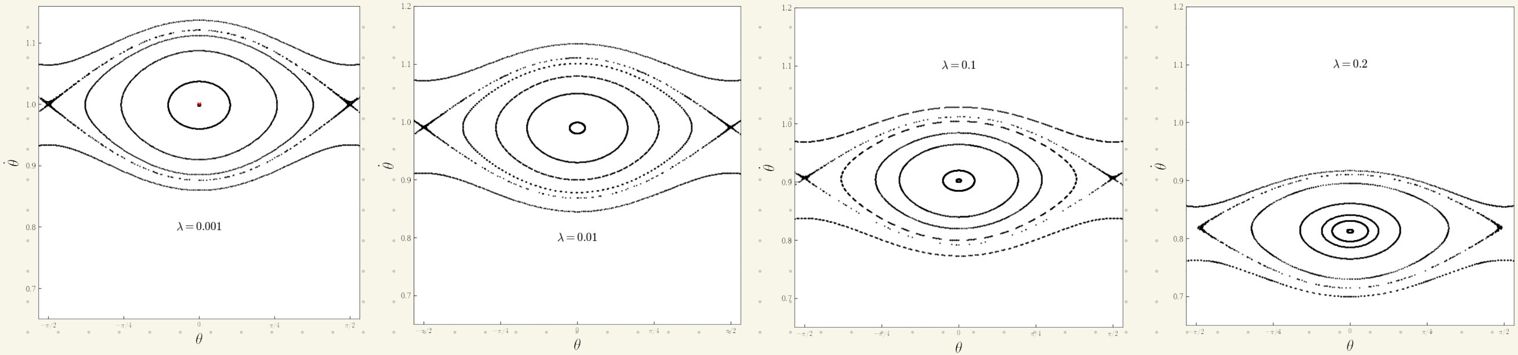


$n=5$

A (CLEAR) ADVANTAGE

Computationally comparable to Euler but with error and structure guarantees

⇒ stronger guarantees for numerical investigations, e.g. on study resonances in the SPIN-ORBIT PROBLEM (Gkolias, Efthymiopoulos, Pucacco, Celletti 2017)



Poincaré surfaces for resonant case for various values of coupling constant to external body torques (left close to conservative, right non-conservative)

A (CLEAR) ADVANTAGE

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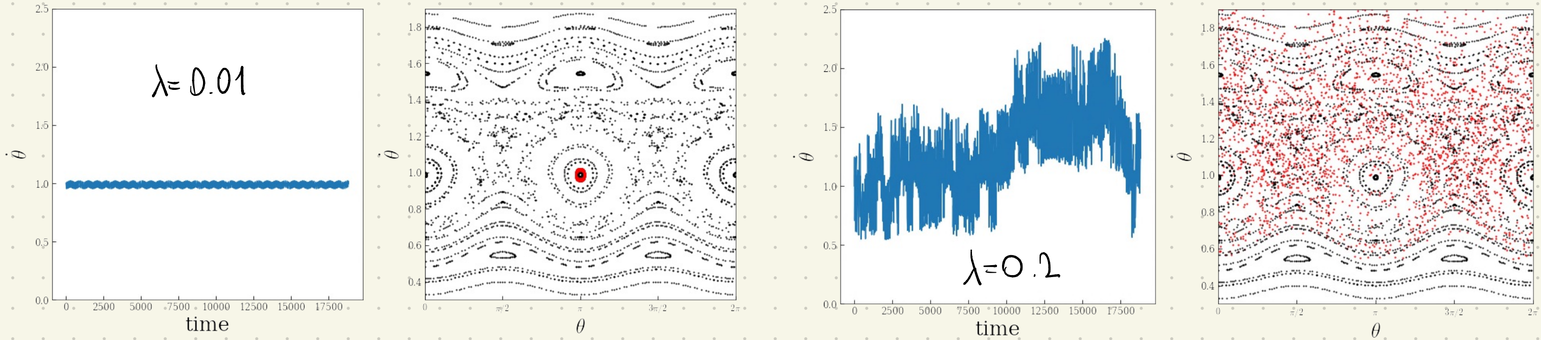
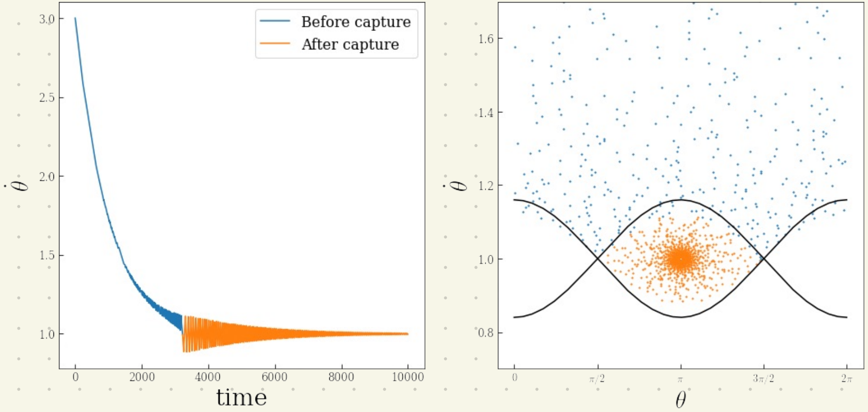


Poincaré surfaces for non-resonant case for various values of coupling constant to external body torques (left close to conservative, right non-conservative)

A (CLEAR) ADVANTAGE

Computationally comparable to Euler but with error and structure guarantees

⇒ stronger guarantees for numerical investigations, e.g. on study resonances in the SPIN-ORBIT PROBLEM (Gkolias, Efthymiopoulos, Pucacco, Celletti 2017)



Confined chaos: a capture into a 1:1 resonance

AN EXAMPLE AWAY FROM CELESTIAL MECHANICS

Van der Pol oscillator

$$\ddot{x} = -x + \varepsilon(1-x^2)\dot{x}$$

$$\begin{cases} \dot{x} = y \\ \dot{y} = -x + \varepsilon(1-x^2)y \end{cases}$$

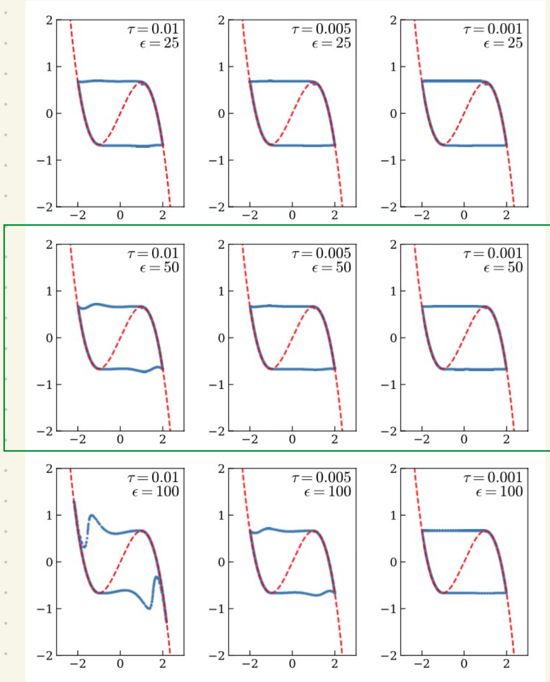
Contact Hamiltonian lift

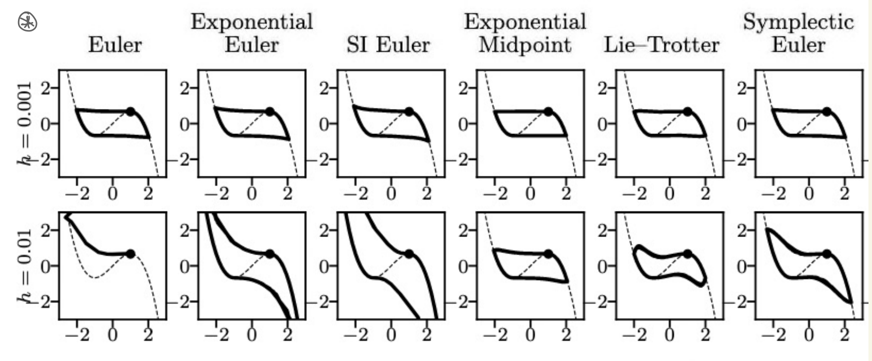
$$H = ps - \varepsilon(1-q^2)s + q$$

$$\begin{cases} \dot{x} = s \\ \dot{s} = -x + \varepsilon(1-x^2)s \\ \dot{p} = -p^2 - 1 + \varepsilon((1-x^2)p - 2xs) \end{cases}$$

If $p_0 = \varepsilon(1-x_0^2) - \frac{x_0}{s_0}$ this is the slope of $\frac{ds}{dx}$ at points $(x(t), s(t))$ of the evolution

VAN DER POL LIMIT CYCLE IN THE STIFF REGIME





⊛ Chen, Roman, Stern – Structure Preserving numerical integrators for Hodgkin-Huxley type systems, SIAM J SCI COMP 2020

FINAL NOTES OF COMPARISON

Contact Variational Integrators

⊕ EXTREMELY STABLE

⊕ HIGHER ACCURACY AT SAME ORDER WRT HAMILTONIAN

⊕ WORKS FOR ANY LAGRANGIAN

⊖ OFTEN IMPLICIT

⊖ MUST BE RE-IMPLEMENTED ON A CASE TO CASE BASIS

Contact Hamiltonian Integrators

⊕ EXPLICIT

⊕ EASY TO IMPLEMENT

⊕ EXTREMELY FAST AT LOW ORDERS

⊖ GETS SLOW AT HIGH ORDERS (> 12)

⊖ ONLY FOR SPLITTING HAMILTONIAN

In both cases, including time dependence is very easy!

CURRENT AND FUTURE WORK

Very active field in rapid growth:

- Hamilton-Jacobi pt of view
- Study of "dissipation laws"
- Aubry-Mather theory
- Numerical methods (statistical mechanics, optimization and fluid mechanics)
- Singular systems, their dynamics and a notion of integrability (work in progress by F. Zadra)
- ...

and thanks for
the patience!

WHAT ABOUT TIME DEPENDENCE?

Modulo some technicalities, all proofs go through in the same way ...

EXAMPLE: DAMPED, DRIVEN OSCILLATOR $\ddot{q} = -\nabla V(q) - \alpha \dot{q} + f(t)$

$$L = \frac{\dot{q}^2}{2} - V(q) - \alpha S + f(t)\, q$$

CONTACT
LEAPFROG
INTEGRATOR

$$\begin{cases} q_{j+1} = q_j + h\left(1 - \frac{h}{2}\alpha\right) p_j - \frac{h^2}{2} V'(q_j) + \frac{h^2}{2} f(t_j) \\ p_{j+1} = \dfrac{\left(1 - \frac{h}{2}\alpha\right) p_j - \frac{h}{2}\left(V'(q_j) + V'(q_{j+1})\right) + \frac{h}{2}\left(f(t_{j+1}) + f(t_j)\right)}{1 + \frac{h}{2}\alpha} \end{cases}$$