Variational integrators for contact Hamiltonian systems

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Discretization in
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Background: symplectic dynamics

Symplectic form ω: closed non-degenerate 2-form on a $2n$-dimensional manifold $\mathcal{M}$

A Hamilton function $H : \mathcal{M} \to \mathbb{R}$ induces a Hamiltonian vector field X_H on $\mathcal{M}$:

$$\iota_{X_H}\omega = \mathrm{d}H$$

In Darboux coordinates $(x_1, \ldots, x_n, p_1, \ldots p_n)$

$$\omega = \sum_i \mathrm{d}p_i \wedge \mathrm{d}x_i$$

The vector field X_H is given by

$$\dot{x} = \frac{\partial H}{\partial p}, \qquad \dot{p} = -\frac{\partial H}{\partial x}.$$

Example. In mechanics, we usually have $H(x,p) = \frac{1}{2}|p|^2 + U(x)$ leading to

$$\dot{x} = p, \qquad \dot{p} = -U'(x)$$

Properties of Hamiltonian systems

The flow of $F_t : \mathcal{M} \to \mathcal{M} : (x(0), p(0)) \mapsto (x(t), p(t))$ of a Hamiltonian vector field preserves the symplectic form,

$$(F_t)^* \omega = \omega,$$

the corresponding volume

$$(F_t)^* \omega^n = \omega^n \qquad = \mathrm{d}p_1 \wedge \ldots \wedge \mathrm{d}p_n \wedge x_1 \wedge \ldots \wedge \mathrm{d}x_n,$$

and the energy,

$$H(x(t), p(t)) = H(x(0), p(0)).$$

If the system has symmetries, then (Noether's theorem) the corresponding generalized momenta are conserved quantities.

Lagrangian mechanics

If we can solve $\dot{x} = \frac{\partial H}{\partial p}$ for p, then solutions to the Hamiltonian equations satisfy a variational principle:

$$\delta \int_0^t \mathcal{L}(x, \dot{x}) \, \mathrm{d}t = 0$$

for variations δx of x leaving the endpoints $x(0)$ and $x(t)$ invariant, where the Lagrangian is $\mathcal{L}(x, \dot{x}) = p\dot{x} - H(x, p)$.

Critical curves are characterized by

$$\forall \delta x : \quad 0 = \int_0^t \frac{\partial \mathcal{L}}{\partial x} \delta x + \frac{\partial \mathcal{L}}{\partial \dot{x}} \delta \dot{x} \, \mathrm{d}t = \int_0^t \left(\frac{\partial \mathcal{L}}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \mathcal{L}}{\partial \dot{x}} \right) \delta x \, \mathrm{d}t$$

$$\Leftrightarrow \frac{\partial \mathcal{L}}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \mathcal{L}}{\partial \dot{x}} = 0 \qquad \text{(Euler-Lagrange equation)}$$

Example. For $H(x, p) = \frac{1}{2}|p|^2 + U(x)$ we find

$$\mathcal{L}(x, \dot{x}) = |\dot{x}|^2 - U(x)$$

leading to the Euler-Lagrange equation $-U'(x) - \ddot{x} = 0$

Geometric discretization

Main idea

Discretization preserving the geometric structure often leads to improved accuracy, especially over long time intervals.

A map $\Phi_h : \mathcal{M} \to \mathcal{M}, \Phi_h(x,p) = (x,p) + \mathcal{O}(h)$ is a consistent discretization of the flow F_t if

$$\Phi_h(x,p) = F^h(x,p) + \mathcal{O}(h^2) \qquad (= (x,p) + \mathcal{O}(h))$$

Φ_h is called symplectic if it preserves ω:

$$(\Phi_h)^* \omega = \omega.$$

An effective way to obtain sympletic integrators is by discretizing the variational principle:

Look for a discrete curve $x_0, x_1, \ldots, x_N$ minimizing the discrete action

$$\sum_i L(x_i, x_{i+1}; h),$$

Properties of symplectic integrators

By definition, a symplectic integrator preserves the symplectic form,

$$(\Phi_h)^* \omega = \omega,$$

and hence the corresponding volume

$$(\Phi_h)^* \omega^n = \omega^n.$$

A symplectic integrator very nearly preserves a modified energy $E_{mod} \approx H$:

$$E_{mod}(\Phi_h^n(x,p)) \approx E_{mod}(x,p)$$

over a time interval of length $\mathcal{O}(e^{-h})$.

If the discretization has symmetries, then there exist conserved generalized discrete momenta.

Linear dissipation

Certain mechanical systems include an isotropic damping term that is linear in the velocity:

$$\ddot{x} = -U'(x) - \alpha \dot{x}, \qquad \alpha \in \mathbb{R},\ x : [0, T] \to \mathbb{R}^n$$

or

$$\dot{x} = p, \qquad \dot{p} = -U'(x) - \alpha p$$

For $\alpha \neq 0$ we do not have conservation of (the usual) energy or symplectic form.

Is there a geometric description of such systems?

Can we use it for geometric discretization?

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Contact geometry

$(2n+1)$-dimensional manifold M.

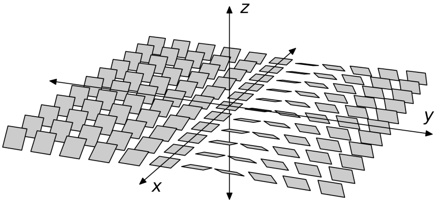
Contact structure

A distribution of hyperplanes $\xi \subset TM$ that is maximally non-integrable: a submanifold that is always tangent to the distribution has dimension at most n.

Locally, such a distribution is given by the kernel of a 1-form η satisfying

$$\eta \wedge (\mathrm{d}\eta)^n \neq 0,$$

called a contact form.



$\mathrm{d}z - y\mathrm{d}x$

Multiplying η by a non-vanishing function does not change the contact structure.

$f : M \to M$ is a contact transformation if $f^*\eta = g\eta$ for some $g : M \to \mathbb{R}$.

Contact Hamiltonian systems

There exist Darboux local coordinates $(x_1, \ldots, x_n, p_1, \ldots, p_n, z)$ such that the contact 1-form can be written as

$$\eta = \mathrm{d}z - p\,\mathrm{d}x \qquad = \mathrm{d}z - \sum_i p_i\,\mathrm{d}x_i.$$

Contact Hamiltonian vector field

$$\mathcal{L}_{X_H}\eta = f_H\eta \qquad \text{and} \qquad \eta(X_H) = -H,$$

where $\mathcal{L}$ is the Lie derivative and $f_H : M \to \mathbb{R}$.
(In terms of the Reeb vector field, $f_H = -R_\eta(H)$.)

For comparison with symplectic mechanics, note that

$$\iota_{X_H}(\mathrm{d}p \wedge \mathrm{d}q) = \iota_{X_H}(\mathrm{d}\eta) = -\mathrm{d}(\iota_{X_H}\eta) + \mathcal{L}_X\eta = \mathrm{d}H + f_H\eta.$$

In Darboux coordinates the contact Hamiltonian equations are

$$\dot{x} = \frac{\partial H}{\partial p}, \qquad \dot{p} = -\frac{\partial H}{\partial x} - p\frac{\partial H}{\partial z}, \qquad \dot{z} = p\frac{\partial H}{\partial p} - H.$$

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Damped mechanical systems

Contact Hamiltonian systems satisfy

$$\frac{\mathrm{d}H}{\mathrm{d}t} = -H\frac{\partial H}{\partial z}$$

so dissipation can occur!

Example. A Hamiltonian of the form

$$H = \frac{1}{2}p^2 + U(x) + \alpha z$$

describes a mechanical system with linear damping:

$$\begin{cases} \dot{x} = p \\ \dot{p} = -U'(x) - \alpha p \\ \dot{z} = p^2 - H. \end{cases}$$

Written as a second order ODE:

$$\ddot{x} = -U'(x) - \alpha \dot{x}.$$

The physical meaning of z will be discussed later.

Contact geometry in thermodynamics

First law for of thermodynamics can be written as

$$\delta U = T\,\delta S + P\,\delta V - \mu\,\delta N$$

i.e. states are constrained within a manifold with tangent spaces in the kernel of

$$\eta = \mathrm{d}U - T\mathrm{d}S + P\mathrm{d}V - \mu\mathrm{d}N$$

Various thermodynamical process can be written as Hamiltonian flows with respect to the contact structure defined by η.

[Mrugała, Nulton, Schön, Salamon. Contact structure in thermodynamic theory. Rep. Math. Phys. 1991]

[Bravetti. Contact geometry and thermodynamics. International Journal of Geometric Methods in Modern Physics, 2018.]

Other applications

- Integrable systems

  [Sergyeyev. New integrable $(3+1)$-dimensional systems and contact geometry. Letters in Mathematical Physics, 2018.]

  [Jovanović B., Jovanović V. Contact flows and integrable systems. Journal of Geometry and Physics, 2015.]

- Optimal control

  [Jóźwikowski, Respondek. A contact covariant approach to optimal control with applications to sub-Riemannian geometry. Math. Control Signals Syst, 2016.]

  [Ohsawa T. Contact geometry of the Pontryagin maximum principle. Automatica, 2015.]

- ...

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Herglotz' variational principle

The contact Hamiltonian equation for z is

$$\dot{z} = p\frac{\partial H}{\partial p} - H \qquad \overset{?}{=} \mathcal{L}$$

Herglotz' variational principle

Lagrangian $\mathcal{L} : TQ \times \mathbb{R} \to \mathbb{R}$.
Given a curve $x : [0, T] \to Q$, define $z : [0, T] \to \mathbb{R}$ by $z(0) = z_0$ and

$$\dot{z}(t) = \mathcal{L}(x(t), \dot{x}(t), z(t))$$

We look for a curve x such that every variation of x that vanishes at the boundary of $[0, T]$ leaves the action $z(T)$ invariant.

If $\mathcal{L}$ does not depend on z we find the classical variational principle:

$$z(T) = \int_0^T \mathcal{L}(x(t), \dot{x}(t)) \, \mathrm{d}t.$$

[Herglotz. Berührungstransformationen Lecture notes, Göttingen, 1930.]

Herglotz' variational principle

A variation δx of x induces a variation δz of z:

$$\dot{z}(t) = \mathcal{L}(x(t), \dot{x}(t), z(t)) \quad \Rightarrow \quad \delta \dot{z} = \underbrace{\frac{\partial \mathcal{L}}{\partial x}\delta x + \frac{\partial \mathcal{L}}{\partial \dot{x}}\delta \dot{x}}_{A(t)} + \underbrace{\frac{\partial \mathcal{L}}{\partial z}}_{\frac{\mathrm{d}B(t)}{\mathrm{d}t}} \delta z.$$

The solution of $\delta \dot{z}(t) = A(t) + \dfrac{\mathrm{d}B(t)}{\mathrm{d}t}\delta z(t)$ is

$$\begin{aligned}
\delta z(T) &= e^{B(T)} \left[\int_0^T A(\tau) e^{-B(\tau)} \,\mathrm{d}\tau + \delta z(0) \right] \\
&= e^{B(T)} \left[\int_0^T \left(\frac{\partial \mathcal{L}}{\partial x}\delta x + \frac{\partial \mathcal{L}}{\partial \dot{x}}\delta \dot{x} \right) e^{-B(\tau)} \,\mathrm{d}\tau + \delta z(0) \right] \\
&= e^{B(T)} \Bigg[\int_0^T \left(\frac{\partial \mathcal{L}}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{x}} + \frac{\partial \mathcal{L}}{\partial z}\frac{\partial \mathcal{L}}{\partial \dot{x}} \right) \delta x \, e^{-B(\tau)} \,\mathrm{d}\tau \\
&\qquad + \frac{\partial \mathcal{L}}{\partial \dot{x}}(T)\delta x(T) \, e^{-B(T)} - \frac{\partial \mathcal{L}}{\partial \dot{x}}(0)\delta x(0) + \delta z(0) \Bigg].
\end{aligned}$$

Herglotz' variational principle

$$\delta z(T) = e^{B(T)}\Bigg[\int_0^T \left(\frac{\partial \mathcal{L}}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{x}} + \frac{\partial \mathcal{L}}{\partial z}\frac{\partial \mathcal{L}}{\partial \dot{x}}\right)\delta x\, e^{-B(\tau)}\,\mathrm{d}\tau + \frac{\partial \mathcal{L}}{\partial \dot{x}}(T)\delta x(T)\, e^{-B(T)} - \frac{\partial \mathcal{L}}{\partial \dot{x}}(0)\delta x(0) + \delta z(0)\Bigg].$$

Variations satisfy $\delta x(0) = \delta x(T) = \delta z(0) = 0$.

Generalized Euler-Lagrange equations

$$\frac{\partial \mathcal{L}}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{x}} + \frac{\partial \mathcal{L}}{\partial z}\frac{\partial \mathcal{L}}{\partial \dot{x}} = 0$$

If instead we restrict to solution curves, but vary the endpoints, we obtain

$$\delta z(T) = \frac{\partial \mathcal{L}}{\partial \dot{x}}(T)\delta x(T) - e^{B(T)}\left[\frac{\partial \mathcal{L}}{\partial \dot{x}}(0)\delta x(0) + \delta z(0)\right]$$

Contact structure

$$\phi_T^*(\mathrm{d}z - p\,\mathrm{d}x) = e^{B(T)}(\mathrm{d}z - p\,\mathrm{d}x)$$

where $p = \frac{\partial \mathcal{L}}{\partial \dot{x}}$ and ϕ_T denotes the flow over the time interval $[0, T]$.

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Discrete Herglotz variational principle

Variational integrator: approximate $\mathcal{L}(x, \dot{x}, z)$ by $L(x_j, x_{j+1}, z_j, z_{j+1}; h)$, where $h > 0$ is the step size.

discrete Herglotz variational principle

Given $x = (x_0, \ldots, x_N) \in Q^{N+1}$ we define $z = (z_0, \ldots, z_N) \in \mathbb{R}^{N+1}$ by $z_0 = 0$ and

$$z_{j+1} - z_j = hL(x_j, x_{j+1}, z_j, z_{j+1}; h)$$

Look for a discrete curve x such that

$$\frac{\mathrm{d}z_{j+1}}{\mathrm{d}x_j} = 0 \qquad \forall j \in \{1, \ldots, N-1\}.$$

Then in particular, $\dfrac{\mathrm{d}z_N}{\mathrm{d}x_j} = 0$ for all $j \in \{1, \ldots, N-1\}$:

variations of x do not affect the final value of z.

Discrete Herglotz variational principle

Discrete generalized Euler-Lagrange equation

$$
\begin{aligned}
0 = {} & \mathrm{D}_2 L(x_{j-1}, x_j, z_{j-1}, z_j) + \mathrm{D}_1 L(x_j, x_{j+1}, z_j, z_{j+1}) \\
& + \frac{h\mathrm{D}_2 L(x_{j-1}, x_j, z_{j-1}, z_j)}{1 - h\mathrm{D}_4 L(x_{j-1}, x_j, z_{j-1}, z_j)} \left(\mathrm{D}_3 L(x_j, x_{j+1}, z_j, z_{j+1}) + \mathrm{D}_4 L(x_{j-1}, x_j, z_{j-1}, z_j) \right).
\end{aligned}
$$

where D_i is the partial derivative w.r.t. the i-th variable.

If L a consistent discretization of a continuous Lagrangian $\mathcal{L}$,

$$
\begin{aligned}
\mathrm{D}_2 L(x_{j-1}, x_j, z_{j-1}, z_j) + \mathrm{D}_1 L(x_j, x_{j+1}, z_j, z_{j+1}) &\approx \frac{\partial \mathcal{L}}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \mathcal{L}}{\partial \dot{x}} \\
\frac{h\mathrm{D}_2 L(x_{j-1}, x_j, z_{j-1}, z_j)}{1 - h\mathrm{D}_4 L(x_{j-1}, x_j, z_{j-1}, z_j)} &\approx \frac{\partial \mathcal{L}}{\partial \dot{x}} \\
\mathrm{D}_3 L(x_j, x_{j+1}, z_j, z_{j+1}) + \mathrm{D}_4 L(x_{j-1}, x_j, z_{j-1}, z_j) &\approx \frac{\partial \mathcal{L}}{\partial z}
\end{aligned}
$$

Contact structure

The discrete generalized Euler-Lagrange equation can be written as

$$\frac{h\mathrm{D}_2 L(x_{j-1}, x_j, z_{j-1}, z_j)}{1 - h\mathrm{D}_4 L(x_{j-1}, x_j, z_{j-1}, z_j)} + \frac{h\mathrm{D}_1 L(x_j, x_{j+1}, z_j, z_{j+1})}{1 + h\mathrm{D}_3 L(x_j, x_{j+1}, z_j, z_{j+1})} = 0$$

Position-momentum formulation

$$F : T^*Q \times \mathbb{R} \mapsto T^*Q \times \mathbb{R} : (x_{j-1}, p_{j-1}, z_{j-1}) \mapsto (x_j, p_j, z_j),$$

where $p_j = p_j^- = p_j^+$ and

$$p_j^- = \frac{h\mathrm{D}_2 L(x_{j-1}, x_j, z_{j-1}, z_j)}{1 - h\mathrm{D}_4 L(x_{j-1}, x_j, z_{j-1}, z_j)},$$
$$p_j^+ = -\frac{h\mathrm{D}_1 L(x_j, x_{j+1}, z_j, z_{j+1})}{1 + h\mathrm{D}_3 L(x_j, x_{j+1}, z_j, z_{j+1})}.$$

The map F is a contact transformation with respect to the 1-form

$$\mathrm{d}z - p\,\mathrm{d}x.$$

All contact maps are variational

Theorem

Iterations of any contact transformation

$$(x_0, p_0, z_0) \mapsto (x_1, p_1, z_1)$$

yield a discrete curve $x = (x_0, \dots, x_N)$ that solves the discrete Herglotz variational principle for some discrete Lagrangian $L(x_j, x_{j+1}, z_j)$.

Proof idea. Like in the symplectic case, every contact transformation has a generating function, which can be used as a discrete Lagrangian. ■

In practice it is beneficial to take L symmetric in z_j and z_{j+1}, but from this Theorem it follows that there is always an equivalent Lagrangian independent of z_{j+1}.

Backward error analysis

Solutions of the difference equations

$$\begin{cases} \dfrac{z_{j+1} - z_j}{h} = L(x_j, x_{j+1}, z_j, z_{j+1}; h) \\ \dfrac{x_{j+1} - 2x_j + x_{j-1}}{h^2} = F(x_{j-1}, x_j, x_{j+1}, z_{j-1}, z_j, z_{j+1}; h). \end{cases}$$

are formally interpolated by solutions of the modified equations

$$\begin{cases} \dot{z} = \mathcal{L}_{\mathrm{mod}}(x, \dot{x}, z, h) = \mathcal{L}(x, \dot{x}, z) + h\mathcal{L}_1(x, \dot{x}, z) + h^2\mathcal{L}_2(x, \dot{x}, z) + \dots \\ \ddot{x} = f_{\mathrm{mod}}(x, \dot{x}, z; h) = f(x, \dot{x}, z) + hf_1(x, \dot{x}, z) + h^2 f_2(x, \dot{x}, z) + \dots \end{cases}.$$

(The power series are usually not convergent. Truncations need to be used to make rigorous statements.)

The modified equations are also a contact system

In particular, $\ddot{x} = f_{\mathrm{mod}}(x, \dot{x}, z; h)$ is the generalized Euler-Lagrange equation of $\mathcal{L}_{\mathrm{mod}}(x, \dot{x}, z, h)$.

Hamiltonian integrators

In many examples, $H(x, p, z) = A(p) + B(x) + Cz$. Then

$$\begin{aligned} X_A &= A'(p)\partial_x + (pA(p) - A(p))\partial_z \\ X_B &= -B'(x)\partial_p - B(x)\partial_z \\ X_{Cz} &= -pC\partial_p - Cz\partial_z, \end{aligned}$$

which are all explicitly integrable:

$$\begin{aligned} \exp(tX_A)(x,p,z) &= (x + tA'(p), p, z + t(pA(p) - A(p))) \\ \exp(tX_B)(x,p,z) &= (x, p - t(B'(x) + B(x)), z + t(pA(p) - A(p))) \\ \exp(tX_C)(x,p,z) &= (x, p - tpC, \exp(Ct)z) \end{aligned}$$

Splitting integrator

$$S_2(h) = \exp\left(\frac{h}{2}X_C\right)\exp\left(\frac{h}{2}X_B\right)\exp(hX_A)\exp\left(\frac{h}{2}X_B\right)\exp\left(\frac{h}{2}X_C\right).$$

As a composition of contact maps, $S_2(h)$ is itself a contact map.

Since it is symmetric, S_2 is a second order integrator.

Hamiltonian integrators

Given a second order contact integrator S_2, higher order contact integrators can be obtained recursively by "Yoshida's trick":

$$S_{2n+2}(h) = S_{2n}(\alpha_n h) S_{2n}(\beta_n h) S_{2n}(\alpha_n h)$$

where $\alpha_n = \frac{1}{2-2^{\frac{1}{2n+1}}}$ and $\beta_n = -\frac{2^{\frac{1}{2n+1}}}{2-2^{\frac{1}{2n+1}}}$.

A more complicated but similar construction for S_2 applies for Hamiltonians

$$H(t,x,p,z) = A(t,p) + B(t,x) + C(t)z$$

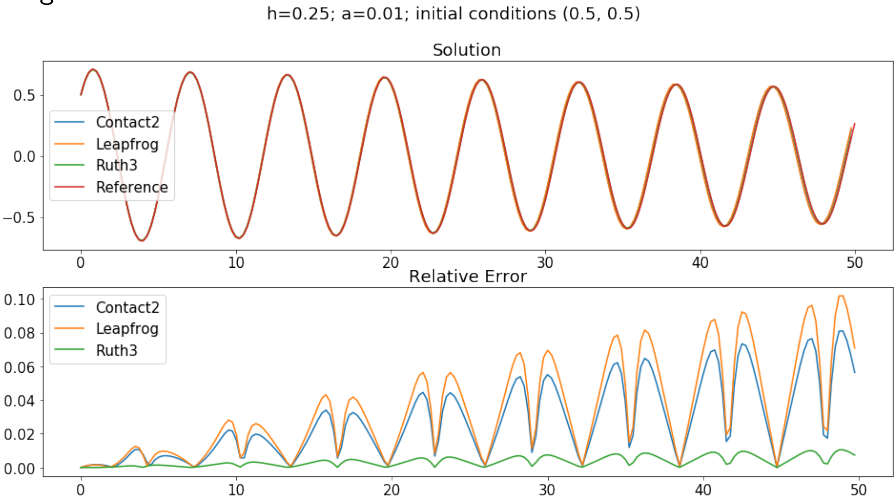
depending explicitly on time.

[Yoshida. Construction of higher order symplectic integrators. Physics letters A, 1990]

Numerical example: harmonic oscillator

$$\mathcal{L} = \frac{1}{2}\dot{x}^2 - \frac{1}{2}x^2 - \alpha z \qquad \Rightarrow \qquad \ddot{x} = -x - \alpha\dot{x}$$

Very small damping: contact integrators comparable to symplectic integrators



Numerical example: harmonic oscillator

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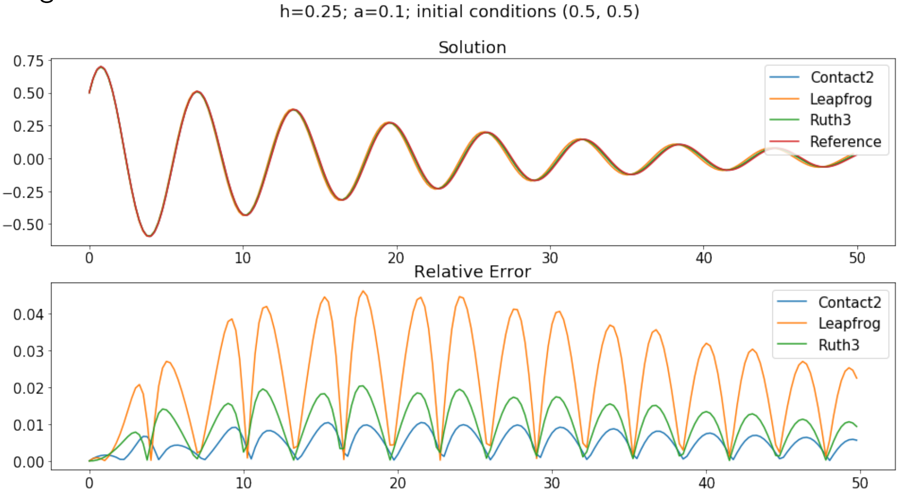
Slightly larger damping: contact integrators better than symplectic integrators



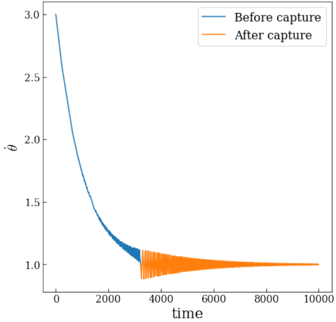
Time-depenent example: spin-orbit mechanics

Flexible satellite in a fixed orbit, experiencing torque from gravity.

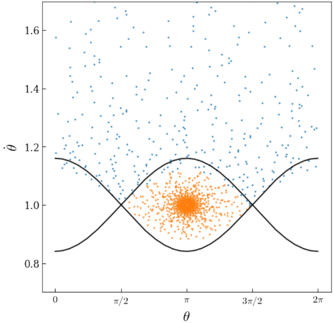
The torque is a time-dependent linear dissipation:

$$H = \frac{p^2}{2} + \frac{N_z(\theta, t)}{C} + \frac{dC}{dt}\frac{1}{C} z \quad \Rightarrow \quad \ddot{\theta} + \frac{dC}{dt}\frac{\dot{\theta}}{C} - \frac{N_z(\theta, t)}{C} = 0.$$

Example: capture into resonance.



Angular velocity decreasing



Poincaré section: angle and angular velocity at fixed point in the orbit

Conclusions

- Contact mechanics is less known than symplectic mechanics, but has significant applications in physics and a similarly rich structure.

- Structure-preserving discretizations for contact systems can be obtained using many of the same ideas as for symplectic systems.

References:

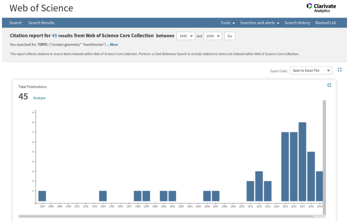
[V, Bravetti, Seri. Contact variational integrators. J Phys A, 2019]

[Bravetti, Seri, V, Zadra. Numerical integration in celestial mechanics: a case for contact geometry. arXiv:1909.02613]

Conclusions

- Contact mechanics is less known than symplectic mechanics, but has significant applications in physics and a similarly rich structure.

  Though it's getting more attention recently...



Number op papers mentioning "contact geometry" and "Hamiltonian" 1987-2019

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