Pseudo-geometric integrators

(Daria Loziienko)

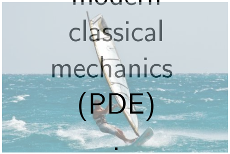
Vladimir Salnikov

CNRS & La Rochelle University

In the previous episodes...

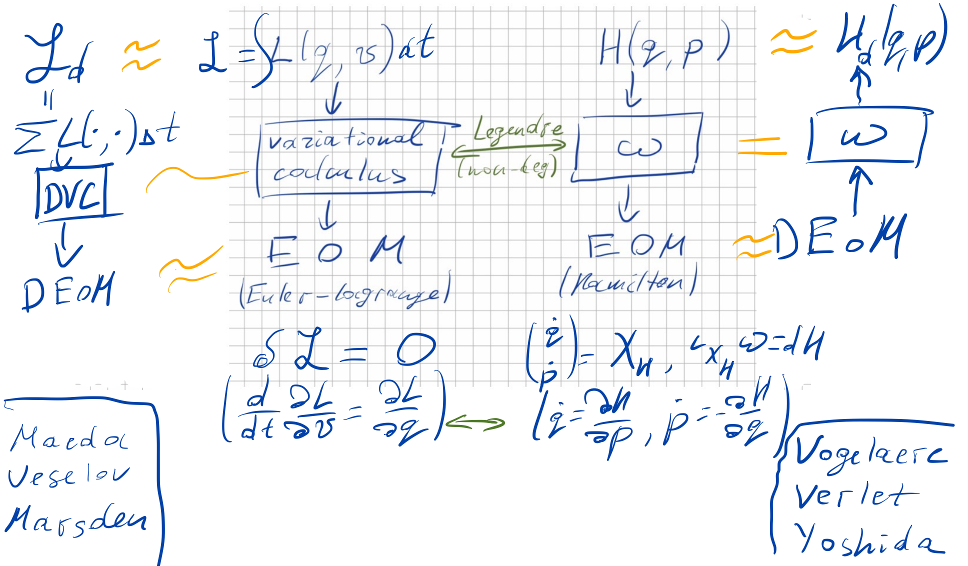
Philosophy:

Geometry encodes the physics of the system

	Mechanical property	Geometric description
 classical classical mechanics (ODE)	conservation of energy	Poisson / symplectic
	symmetries	Lie groups/algebras, Cartan moving frames
	dissipation / interaction power balance; constraints	(almost) Dirac
	control	(singular) foliations
 modern classical mechanics (PDE)	conservation of energy	multisymplectic
	symmetries	Cartan moving frames
	dissipation / interaction	Stokes–Dirac
	$rot(grad) = 0$, $div(rot) = 0$	$d^2 = 0$ – DEC
	control	foliations

Preserving this geometry in computations is fruitful

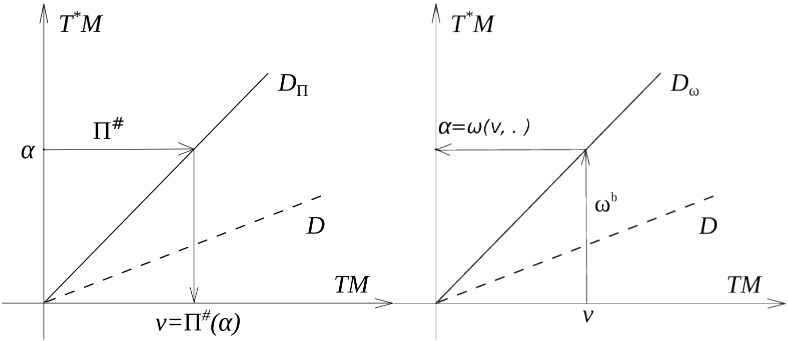
Classical story in modern language



Geometry behind: Courant algebroids, Dirac structures

On $\mathbb{T}M = TM \oplus T^*M$ (or more generally $E \oplus E^*$)
Symmetric pairing: $< v \oplus \eta, v' \oplus \eta' >= \eta(v') + \eta'(v)$,
Dorfman bracket: $[v \oplus \eta, v' \oplus \eta']_D = [v, v']_{\mathrm{Lie}} \oplus (\mathcal{L}_v \eta' - \mathrm{d}\eta(v'))$.

A *Dirac structure* $\mathcal{D}$ is a maximally isotropic (Lagrangian) subbundle of $\mathbb{T}M$ closed w.r.t. $[\cdot,\cdot]_D$



$\mathcal{D}_\Pi = graph(\Pi^\sharp) = \{(\Pi^\sharp \alpha, \alpha)\}$ $\qquad$ $\mathcal{D}_\omega = graph(\omega^\flat) = \{(v, \iota_v \omega)\}$

Dirac paths

Theorem 1. Let $D \subset \mathbb{T}M$ be a Dirac structure over M, $H \in C^\infty(M)$ be a Hamiltonian function and γ a path on M.

Assume that the basic 2-class $[\omega_D]$ vanishes, and let $\theta \in \Gamma(D^*)^{hor}$ be such that $d_D\theta = \omega_D$, then the following statements are equivalent:

(i) The path γ is a Hamiltonian curve, i.e. $(\dot\gamma(t), dH_{\gamma(t)}) \in D$ for all t.

(ii) All Dirac paths $\zeta : I \to D$ over γ (i.e. $\rho(\zeta) = \dot\gamma$) are critical points among the Dirac paths with the same end points of the following functional:

$$\zeta \mapsto \int_I \left(\theta_{\gamma(t)}(\zeta(t)) + H(\gamma(t))\right) dt \tag{1}$$

E.g.
$D = \text{graph } \omega$
$\omega = d(p\,dq)$

$\downarrow (-p\dot q + H)$

Implicit Lagrangian systems with magnetic terms

Theorem 2. Let $D \subset \mathbb{T}Q$ be a Dirac structure and $L : TQ \to \mathbb{R}$ a Lagrangian. Assume that the 2-form $\omega_D \in \Gamma(\Lambda^2 D^*)^{hor}$ admits a basic primitive $\theta \in \Gamma(D^*)^{hor}$. Then for $q : I \to Q$ the following are equivalent:

a) There exists a Dirac path $\zeta : I \to D$ such that $\rho(\zeta) = \dot{q}$ which is the critical point among Dirac paths with the same end points of

$$\int_I (L(\rho(\zeta(t))) + \theta(\zeta(t)))dt. \tag{2}$$

b) For all $t \in I$, the following condition holds.

$$\left(\frac{\partial}{\partial t} \mathbb{F}L(\dot{q}(t)), \mathcal{D}_{\dot{q}(t)} L \right) \in \mathbb{D} = e^{\Omega} \pi^! D. \tag{3}$$

Example (Holonomic constraints)

Let $F \subset TQ$ be a regular foliation, and $F^\circ \subset T^*Q$ its annihilator. The Dirac structure $D = F \oplus F^\circ$ always admits a basic potential, as the 2-form in $\Lambda^2 D^*$ is zero (there is no magnetic term). Then $\pi^! D$ is the Dirac structure associated to the pullback foliation $\pi^{-1}(F)$ and

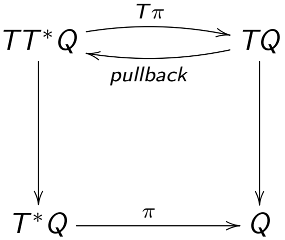
$$e^\Omega \pi^! D = \{(w, \alpha) \in TT^*Q \oplus T^*T^*Q \mid \pi_*(w) \in F, \alpha - \Omega^\flat w \in \pi^{-1}(F)^\circ\}$$

Let $L : TQ \to \mathbb{R}$ be a Lagrangian. Then Theorem 2 yields that the integral curves of any implicit Lagrangian system $(X, \mathcal{D}L)$ for $e^\Omega \pi^! D$ are critical points of L among curves that are tangent to F. The condition (3) (belonging to $\mathbb{D}$) translates directly to the Euler-Lagrange equations for a system subject to holonomic constraints, which are classically spelled-out using the Lagrange multipliers.

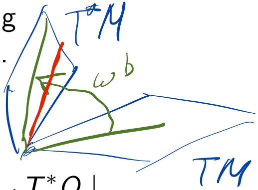
Application. Implicit Lagrangian systems / constraints

Tulczyjew (70's), H. Yoshimura, J.E. Marsden (2006).

1. Geometry:



$\Delta_Q \subset TQ$ constraint distribution:
$\Delta_Q(q) = \{v \in T_qQ \ |\omega^a_q(v) = 0\}$.
$\Delta_{T^*Q} \subset TT^*Q$ – preimage of Δ_Q, and $\Delta^0_{T^*Q}$ its annihilator.
The canonical symplectic form Ω on T^*Q defines a mapping $\Omega^\flat \colon TT^*Q \to T^*T^*Q$.



Almost Dirac structure:

$$\mathbb{D}_{\Delta_Q}((q,p)) = \{(w,\alpha) \in T_{(q,p)}T^*Q \times T^*_{(q,p)}T^*Q \ | \quad w \in \Delta_{T^*Q}, \quad \alpha - \Omega^\flat w \in \Delta^0_{T^*Q})\} \qquad (2)$$

2. Dynamics. $L\colon TQ \to \mathbb{R}$ – Lagrangian.
Its differential defines a mapping $\mathrm{d}L\colon TQ \to T^*TQ$.
There are symplectomorphisms $\Omega^\flat\colon TT^*Q \to T^*T^*Q$ as well as $\kappa_Q\colon TT^*Q \to T^*TQ$, then $\gamma_Q := \Omega^\flat \circ \kappa_Q^{-1}\colon T^*TQ \to T^*T^*Q$.

Define the *Dirac differential* $\mathcal{D}L := \gamma_Q \circ \mathrm{d}L\colon TQ \to T^*T^*Q$.
Locally: $(q, v) \to (q, \frac{\partial L}{\partial v}, -\frac{\partial L}{\partial q}, v)$.

Consider a partial vector field X, i.e. a mapping
$X\colon \Delta_Q \oplus Leg(\Delta_Q) \subset TQ \oplus T^*Q \to TT^*Q$.
It can be viewed as $X(q, p)$, where p is given by the Legendre transform, and v is in the constraint distribution.

3. All together An *implicit Lagrangian system* is a triple (L, Δ_Q, X), s.t. $(X, \mathcal{D}L) \in \mathbb{D}_{\Delta_Q}$ (eq. 2)

Locally this means $p = \frac{\partial L}{\partial v},\ \dot{q} = v,\ \dot{q} \in \Delta$, and
$\dot{p} - \frac{\partial L}{\partial q} \in \Delta^0(q) \Leftrightarrow \dot{p} - \frac{\partial L}{\partial q} = \sum_a \lambda_a \alpha^a$.

How to discretize?

$$\begin{cases} \alpha^a(v) = 0, \quad a = 1, \dots, m. \\ \mathbf{p} = \frac{\partial L}{\partial \mathbf{v}}, \qquad \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} - \frac{\partial L}{\partial \mathbf{q}} = \sum_{a=1}^{m} \lambda_a \alpha^a. \end{cases}$$

The discrete Lagrangian $L_d = \Delta t \; L(\mathbf{q}^n, \mathbf{v}^n)$.

Discrete equations:

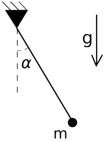
$$< \alpha_d^a, \mathbf{v}^n >= 0, \quad a = 1, \dots, m; \quad \mathbf{p}^{n+1} = \frac{1}{\Delta t} \frac{\partial L_d}{\partial \mathbf{v}^n}$$

$$\mathbf{p}^n - \frac{1}{\Delta t} \frac{\partial L_d}{\partial \mathbf{v}^n} + \frac{\partial L_d}{\partial \mathbf{q}^n} = \sum_{a=1}^{m} \lambda_a \frac{\partial < \alpha_d^a, \mathbf{v}^n >}{\partial \mathbf{v}^n}$$

Explicitly $\mathbf{p}^n$ and $\mathbf{p}^{n+1}$, and $\mathbf{v}^n$ – approximates the velocity, containing $\mathbf{q}^n$, e.g. $\mathbf{v}^n := \dfrac{\mathbf{q}^{n+1} - \mathbf{q}^n}{\Delta t}$ or $\mathbf{v}^n := \dfrac{\mathbf{q}^{n+1} - \mathbf{q}^{n-1}}{2\Delta t}$.

$2d + m$ equations for $2d + m$ unknowns.

Baby example



Description of Δ_Q and Δ_{T^*Q}:
$Q = \mathbb{R}^2$,
Constraint $\phi(x, y) := x^2 + y^2 - l^2 = 0$.
The distribution Δ_Q is generated by $\xi = y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}$.
in the kernel of $\psi = \mathrm{d}\phi = 2(x\mathrm{d}x + y\mathrm{d}y)$.

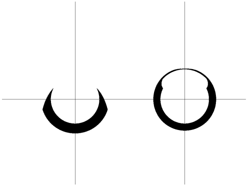
Lagrangian differential and Legendre transform.
The Lagrangian is $L = \frac{m}{2}(\dot{x}^2 + \dot{y}^2) - mgy$. The associated Lagrangian differential
$\mathcal{D}L = (q, \frac{\partial L}{\partial v}, -\frac{\partial L}{\partial q}, v) = ((x, y), (m\dot{x}, m\dot{y}), (0, mg), (\dot{x}, \dot{y}))$.

All together

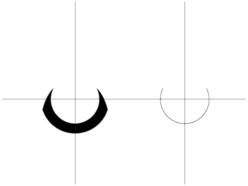
$$\dot{q} \in \Delta_Q, \qquad p = \frac{\partial L}{\partial v}$$
$$\dot{q} = v, \qquad \dot{p} - \frac{\partial L}{\partial q} \in \Delta_Q^0$$

$$x\dot{x} + y\dot{y} = 0$$
$$\ddot{x} = \lambda x$$
$$\ddot{y} = -mg + \lambda y$$

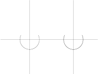
Simulations: Dirac 1 vs Euler



Simulations : Dirac 1 vs Dirac 2

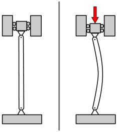


Simulations : Dirac 2 vs All Stars

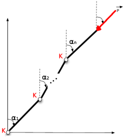


Dirac order 1(M.Leok, T.Ohsawa)
$\rightarrow$ 0.952115
Dirac order 2 (V.S.)
$\rightarrow$ 0.00204053
Trapezium 2(implicit and cheating)
$\rightarrow$ 0.0128399
Adams–Bashforth 3 (cheating)
$\rightarrow$ 0.000136601
Runge–Kutta 4 (still cheating)
$\rightarrow 9.4 \cdot 10^{-8}$

Real example



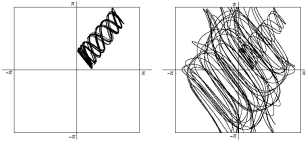
Buckling



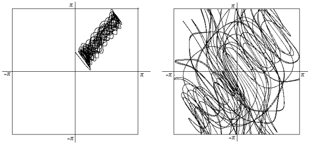
Ziegler–Bigoni system

Application. Geometric degree of nonconservativity (cf. J.Lerbet, M.Aldowaji, N.Challamel, O.Kirillov, F.Nicot, F.Darve)

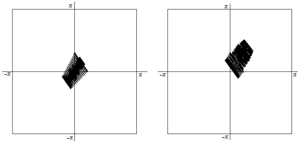
Simulations : Dirac 2 vs Dirac 1



Simulations : Dirac vs classical methods



Simulations : Dirac 1 vs Dirac 2



Exercise: Compare with Jean Lerbet!

Details:

- V.S., A.Hamdouni, From modelling of systems with constraints to generalized geometry and back to numerics, ZAMM 2019;
- D. Razafindralandy, V.S., A. Hamdouni, A. Deeb, Some robust integrators for large time dynamics, AMSES, 2019.

How to honestly discretize? What is wrong?

Symplectic Euler for $\dot{q} = H_p, \quad \dot{p} = -H_q$

$$\begin{aligned} q^{n+1} &:= q^n + \Delta t \cdot H_p^n \\ p^{n+1} &:= p^n - \Delta t \cdot H_q^{n+1} \end{aligned}$$

Dirac methods for $\alpha^a(v) = 0, \quad \mathbf{p} = \frac{\partial L}{\partial \mathbf{v}}, \quad \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} - \frac{\partial L}{\partial \mathbf{q}} = \sum_{a=1}^{m} \lambda_a \alpha^a.$

$$< \alpha_d^a, \mathbf{v}^n >= 0, \quad a = 1, \ldots, m; \quad \mathbf{p}^{n+1} = \frac{1}{\Delta t} \frac{\partial L_d}{\partial \mathbf{v}^n}$$

$$\mathbf{p}^n - \frac{1}{\Delta t} \frac{\partial L_d}{\partial \mathbf{v}^n} + \frac{\partial L_d}{\partial \mathbf{q}^n} = \sum_{a=1}^{m} \lambda_a \frac{\partial < \alpha_d^a, \mathbf{v}^n >}{\partial \mathbf{v}^n}$$

$$\mathbf{v}^n := \frac{\mathbf{q}^{n+1} - \mathbf{q}^n}{\Delta t} \text{ or } \mathbf{v}^n := \frac{\mathbf{q}^{n+1} - \mathbf{q}^{n-1}}{2\Delta t}$$

Wishful thinking and reality

AKA geometric integrators

Letter to Ded Moroz* (want to be theorem)
We discretize the equations in such a way that the Dirac structure is preserved exactly, hence the physical properties are also preserved exactly.

AKA pseudo-geometric integrators of order (*, p)

Reply (actual theorem)
We discretize the equations in such a way that the Dirac structure is preserved up to some power of Δt, hence the physical properties are also preserved up to some (other) power of Δt.

p

Gifts (algorithm)
– Write a (possibly implicit) Runge–Kutta method for each type of variables, with different undetermined coefficients.
– Suppose at the n-th step the variables belong to the Dirac structure, compute the error at the $(n+1)$-st step
– Maximize the order of the error by a good choice of coefficients.

* Santa Claus

Theorem. Consider $q_{n+1} = q_n + hb_1 l_1 + hb_2 l_2$,
$p_{n+1} = p_n + h\tilde{b}_1 \tilde{l}_1 + h\tilde{b}_2 \tilde{l}_2$, $\quad v_{n+1} = v(v_n + h\bar{b}_1 \bar{l}_1 + h\bar{b}_2 \bar{l}_2)$, where
$l_1 = v(v_n + h\bar{a}_{11}\bar{l}_1 + h\bar{a}_{12}\bar{l}_2)$...

1. The numerical method above is of **second order** provided that
$b_1 + b_2 = 1$, $\tilde{b}_1 + \tilde{b}_2 = 1$, $\tilde{b}_1\tilde{a}_{11} + \tilde{b}_2\tilde{a}_{21} + \tilde{b}_1\tilde{a}_{12} + \tilde{b}_2\tilde{a}_{22} = \frac{1}{2}$,
$b_1 a_{11} + b_2 a_{21} + b_1 a_{12} + b_2 a_{22} = \frac{1}{2}$.

2. It preserves the Legendre transformation at least up to the **third order** provided that $b_1 + b_2 = \tilde{b}_1 + \tilde{b}_2 = 1$,
$\tilde{b}_1 a_{11} + \tilde{b}_2 a_{21} + \tilde{b}_2 a_{22} + \tilde{b}_1 a_{12} = \frac{1}{2}$,
$\tilde{b}_1 \bar{a}_{11} + \tilde{b}_2 \bar{a}_{21} + \tilde{b}_2 \bar{a}_{22} + \tilde{b}_1 \bar{a}_{12} = \frac{1}{2}$.

3. It preserves the constraints at least up to the **third order** provided that $\tilde{b}_1\tilde{a}_{11} + \tilde{b}_2\tilde{a}_{21} + \tilde{b}_1\tilde{a}_{12} + \tilde{b}_2\tilde{a}_{22} = \frac{1}{2}$,
$b_1 a_{11} + b_2 a_{21} + b_1 a_{12} + b_2 a_{22} = \frac{1}{2}$,
$b_1 \bar{a}_{11} + b_1 \bar{a}_{12} + b_2 \bar{a}_{21} + b_2 \bar{a}_{22} = \frac{1}{2}$,
$\bar{b}_1 a_{11} + \bar{b}_1 a_{12} + \bar{b}_2 a_{21} + \bar{b}_2 a_{22} = \frac{1}{2}$,
$\bar{b}_1 \bar{a}_{11} + \bar{b}_1 \bar{a}_{12} + \bar{b}_2 \bar{a}_{21} + \bar{b}_2 \bar{a}_{22} = \frac{1}{2}$,
$b_1 + b_2 = 1$, $\tilde{b}_1 + \tilde{b}_2 = 1$, $\bar{b}_1 + \bar{b}_2 = 1$.

pseudo-Dirac of order (2, 3)

Pendulum

Step	Method	Energy error	Constraint error	time,sec
10^{-2}	RKD-2 (1)	10^{-2}	10^{-2}	1.64
10^{-3}	RKD-2 (1)	10^{-4}	10^{-5}	7.27
10^{-4}	RKD-2 (1)	10^{-6}	10^{-7}	80.36
10^{-2}	RKD-2 (2)	10^{-2}	10^{-3}	1.63
10^{-3}	RKD-2 (2)	10^{-4}	10^{-5}	6.64
10^{-4}	RKD-2 (2)	10^{-6}	10^{-7}	50.30
10^{-2}	Dirac-2	13.26	2.72×10^{-2}	0.25
10^{-3}	Dirac-2	1.8	1.5×10^{-3}	2.24
10^{-4}	Dirac-2	1.9×10^{-1}	1.4×10^{-4}	24.63

Chaplygin sleigh

Step	Method	Energy error	Constraint error	time,sec
10^{-2}	RKD-2 (1)	7×10^{-6}	5×10^{-6}	23.77
10^{-3}	RKD-2 (1)	7×10^{-8}	5×10^{-8}	95.84
10^{-4}	RKD-2 (1)	7×10^{-10}	5×10^{-10}	700.14
10^{-2}	RKD-2 (2)	7×10^{-6}	5×10^{-6}	11.75
10^{-3}	RKD-2 (2)	7×10^{-8}	5×10^{-8}	59.95
10^{-4}	RKD-2 (2)	7×10^{-10}	5×10^{-10}	416.48
10^{-2}	Dirac-2	7.9×10^{-3}	10^{-2}	1.62
10^{-3}	Dirac-2	7.6×10^{-4}	10^{-3}	18.05
10^{-4}	Dirac-2	1.2×10^{-4}	10^{-4}	223.83

Good remarks

1. We recover symplectic Runge-Kutta methods

2. There are a lot of coefficients, but this is algorithmic —> paper in J. of Programming and Computer Software

Other remarks / work in progress

1. We understood why Marsden inspired method was not really geometric.
1.bis it was pseudo-geometric of order (1,2)

2. Dirac-2 was not much better: something like order (1,2 ; 2,3)

3. TODO: I still want it to be (honestly) variational

Trugarez deoc'h evit bezañ bet o selaou ac'hanon!