Short talk: High-order geometric methods for nonholonomic mechanical systems.

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Mechanical systems

Mechanical systems

- Described via Lagrangian or Hamiltonian formulation
- Built-in geometric properties (Manifold structure of configuration space, symplecticity)
- Built-in conservation laws due to symmetries (Noether theorem)

Question 1

Can we find numerical methods that respect / preserve these?

Mindful integration

As it turns out, mostly yes.

Structure preserving algorithms ([Hairer], [Sanz-Serna], [Munthe-Kaas], ...)

- We can try to respect the manifold structure of the configuration space.
- We can preserve at least first or second order invariants (energy, symplectic form).

For mechanical systems we take special interest in a set of constant step-size methods called *symplectic methods*.

Symplectic integrators

Why do we like symplectic integrators?

- Good qualitative and quantitative behaviour.

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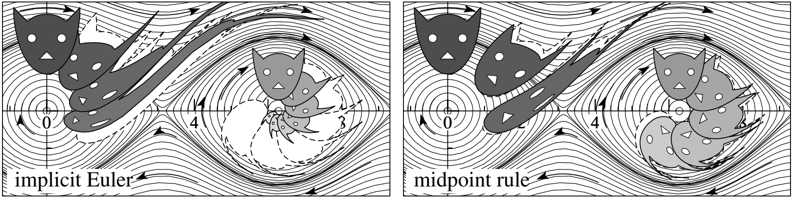

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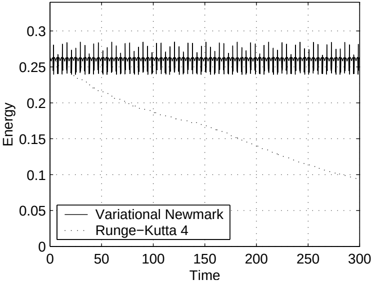

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How come energy behaves so well?

Theorems ([Moser], [Benettin & Giogilli], [Tang], [Murua]...) warrant that symplectic integrators are integrating exactly some existing Hamiltonian system that is *close* to the original one.

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Question 2

How do we build them?

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Generating symplectic integrators easily

Variational integrators are always symplectic.

Idea ([Veselov], [Suris], [Marsden & West]...)

- Substitute continuous state space with discrete one.

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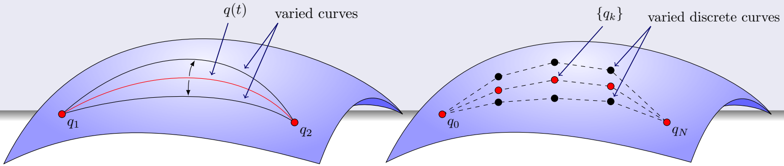

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- Substitute continuous state space with discrete one.
- Build a discrete analogue of Hamilton's principle.

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- Derive equations of motion and conservations from the principle.

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- Substitute continuous state space with discrete one.
- Build a discrete analogue of Hamilton's principle.
- Derive equations of motion and conservations from the principle.

Discrete equations of motion = Difference equations (a.k.a. **our integrator**).

Building blocks

Exact discrete Lagrangian

$$L_d^e(q_0, q_1) = \int_0^h L(q(\tau), \dot{q}(\tau))\mathrm{d}\tau$$

where $q(t)$ solution of the Euler-Lagrange eqs. with fixed boundary values $q(0) = q_0$, $q(h) = q_1$.

Approximation. Discrete Lagrangian

L_d approx. of order r if $\exists C_1 > 0, h_1 > h > 0$ s.t.

$$\|L_d(q(0), q(h)) - L_d^e(q(0), q(h))\| \leq C_1 h^{r+1}$$

Discrete principle and governing equations

Discrete Hamilton's principle

Discrete curve $q_d = \{q_i\}_{i=0}^{N}$ solution of the discrete Lagrangian system $\Leftrightarrow$ critical point of the functional:

$$\mathcal{J}_d(q_d) = \sum_{k=0}^{N-1} L_d(q_k, q_{k+1})$$

Discrete Euler-Lagrange (DEL) equations

$$D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) = 0, \forall k = 1, ..., N-1$$

Connection with Hamiltonian mechanics

Discrete fibre derivatives

$$
\begin{array}{rrcl}
\mathbb{F}L_d^+ : & Q \times Q & \to & T^*Q \\
 & (q_0, q_1) & \mapsto & (q_1, p_1 \equiv D_2 L_d(t_0, q_0, q_1)) \\
\mathbb{F}L_d^- : & Q \times Q & \to & T^*Q \\
 & (q_0, q_1) & \mapsto & (q_0, p_0 \equiv -D_1 L_d(t_0, q_0, q_1))
\end{array}
$$

These provide interpretation of DEL equations as matching of momenta:

$$
p_k^- = D_2 L_d(q_{k-1}, q_k) = -D_1 L_d(q_k, q_{k+1}) = p_k^+
$$

Diagram and convergence

$$
\begin{array}{lccccc}
Q \times Q : & & (q_0, q_1) & \xrightarrow{\;F_{L_d}\;} & (q_1, q_2) & \\
& \swarrow^{\mathbb{F}L_d^-} & & \searrow^{\mathbb{F}L_d^+} \; \swarrow^{\mathbb{F}L_d^-} & & \searrow^{\mathbb{F}L_d^+} \\
T^*Q : & (q_0, p_0) & \xrightarrow{\;\widetilde{F}_{L_d}\;} & (q_1, p_1) & \xrightarrow{\;\widetilde{F}_{L_d}\;} & (q_2, p_2)
\end{array}
$$

Theorem. Variational error [Marsden & West, Patrick & Cuell]

If $\widetilde{F}_{L_d}$ Hamiltonian map of an order r discrete Lagrangian L_d, then

$$\widetilde{F}_{L_d} = \widetilde{F}_{L_d^e} + \mathcal{O}(h^{r+1}).$$

The starting point

Hamilton-Pontryagin action

$(q, v, p) : [a, b] \subset \mathbb{R} \to TQ \oplus T^*Q$, $C^1([a, b])$ curve with $C^2([a, b])$ base component and fixed boundary values $q(a) = q_a$, $q(b) = q_b$.

$$\mathcal{J}_{\mathcal{HP}}(q, v, p) = \int_0^h [L(q(t), v(t)) + \langle p(t), \dot{q}(t) - v(t) \rangle] \, \mathrm{d}t$$

Dynamical equations

$$\begin{aligned} \frac{\mathrm{d}p(t)}{\mathrm{d}t} &= D_1 L(q(t), v(t)), \\ p(t) &= D_2 L(q(t), v(t)), \\ \frac{\mathrm{d}q(t)}{\mathrm{d}t} &= v(t), \quad \forall t \in [0, h]. \end{aligned}$$

Discretizing the action

Discrete Hamilton-Pontryagin action

$$(\mathcal{J}_{\mathcal{HP}})_d = \sum_{k=0}^{N-1} \sum_{i=1}^{s} h b_i \left[L\left(Q_k^i, V_k^i\right) + \left\langle p_k^i, \frac{Q_k^i - q_k}{h} - \sum_{j=1}^{s} a_{ij} V_k^j \right\rangle \right.$$
$$\left. + \left\langle p_{k+1}, \frac{q_{k+1} - q_k}{h} - \sum_{j=1}^{s} b_j V_k^j \right\rangle \right]$$

where (a_{ij}, b_j) coefficients of a Runge-Kutta (RK) method.

Discrete dynamics in T^*Q

Discrete dynamical equations: Symplectic partitioned RK methods

$$q_{k+1} = q_k + h\sum_{j=1}^{s} b_j V_k^j, \quad p_{k+1} = p_k + h\sum_{i=1}^{s} \hat{b}_j W_k^j,$$

$$Q_k^i = q_k + h\sum_{j=1}^{s} a_{ij} V_k^j, \quad P_k^i = p_k + h\sum_{j=1}^{s} \hat{a}_{ij} W_k^j,$$

$$W_k^i = D_1 L(Q_k^i, V_k^i), \quad P_k^i = D_2 L(Q_k^i, V_k^i),$$

where $(\hat{a}_{ij}, \hat{b}_j)$ satisfy $b_i\hat{a}_{ij} + \hat{b}_j a_{ji} = b_i\hat{b}_j$ and $\hat{b}_i = b_i$.

Discrete dynamics in TQ

Discrete dynamical equations: Symplectic partitioned RK methods

$$q_{k+1} = q_k + h\sum_{j=1}^{s} b_j V_k^j, \quad p_{k+1} = p_k + h\sum_{i=1}^{s} \hat{b}_j W_k^j,$$

$$Q_k^i = q_k + h\sum_{j=1}^{s} a_{ij} V_k^j, \quad P_k^i = p_k + h\sum_{j=1}^{s} \hat{a}_{ij} W_k^j,$$

$$W_k^i = D_1 L(Q_k^i, V_k^i), \quad P_k^i = D_2 L(Q_k^i, V_k^i),$$

$$p_k = D_2 L(q_k, v_k), \quad p_{k+1} = D_2 L(q_{k+1}, v_{k+1}),$$

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Nonholonomic mechanics

Nonholonomic Lagrangian system

(L, Q, N) with N, constrain manifold with $i_N : N \hookrightarrow TQ$. Locally described by null-set of $\Phi : TQ \to \mathbb{R}^m$, $m = \mathrm{codim}_{TQ} N$.

Dynamical equations

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}^i}\right) - \frac{\partial L}{\partial q^i} &= \left\langle \lambda, \frac{\partial \Phi}{\partial \dot{q}^i} \right\rangle, \\ \Phi(q, \dot{q}) &= 0 \end{cases} \qquad \forall i = 1, \ldots, n$$

NON-VARIATIONAL (NOR SYMPLECTIC)!! Obtained via Chetaev's principle. λ are Lagrange multipliers.

Should we throw away our variational integrators?

Discrete nonholonomic mechanics

No, we can still build from the variational substrate. Previous attempts by [de León, Martín de Diego & Santamaría], [Cortés & Martínez], [Ferraro, Iglesias & Martín de Diego], [Jay]...

Idea

Somehow construct discrete nonholonomic fibre derivatives $\mathbb{F}\left(L_d^N\right)^{\pm} : Q \times Q \to M$, where $M = \mathbb{F}L^N(N)$ and $L^N = L \circ i_N$.

Augmented point of view

Easier to build $\Gamma_d^{\pm} : Q \times \Lambda \times Q \times \Lambda \to T^*Q \times \Lambda$, where $\Lambda \cong \mathbb{R}^m$, and find λ_0, λ_1 s.t. $\Gamma_d^{\pm}(q_0, \lambda_0, q_1, \lambda_1) \in T^*Q|_M \times \Lambda$.

Discrete nonholonomic mechanics II

For a certain family of RK methods (a_{ij}, b_j) (Lobatto-type):

Nonholonomic integrator

$$
\begin{aligned}
q_{k+1} &= q_k + h\sum_{i=1}^{s} b_i V_k^i, & p_{k+1} &= p_k + h\sum_{i=1}^{s} \hat{b}_i W_k^i,\\
Q_k^i &= q_k + h\sum_{j=1}^{s} a_{ij} V_k^j, & P_k^i &= p_k + h\sum_{j=1}^{s} \hat{a}_{ij} W_k^j,\\
W_k^i &= D_1 L(Q_k^i, V_k^i) + \left\langle \Lambda_k^i, D_2\Phi(Q_k^i, V_k^i)\right\rangle, & P_k^i &= D_2 L(Q_k^i, V_k^i),\\
q_k^i &= Q_k^i, & p_k^i &= p_k + h\sum_{j=1}^{s} a_{ij} W_k^j,
\end{aligned}
$$

$$\Psi(q_k^i, p_k^i) = 0$$

where $(\hat{a}_{ij}, \hat{b}_j)$ satisfy $b_i \hat{a}_{ij} + \hat{b}_j a_{ji} = b_i \hat{b}_j$ and $\hat{b}_i = b_i$ and $\Psi = \Phi \circ \mathbb{F}L^{-1}$.

This generates a well-defined nonholonomic Hamiltonian flow $\widetilde{F}_{L_d}^{\Lambda} : T^*Q|_M \times \Lambda \to T^*Q|_M \times \Lambda, (q_0, p_0, \lambda_0) \mapsto (q_1, p_1, \lambda_1)$.

Discrete nonholonomic mechanics III

Nonholonomic integrator

$$q_{k+1} = q_k + h\sum_{i=1}^{s} b_i V_k^i, \qquad p_{k+1} = p_k + h\sum_{i=1}^{s} \hat{b}_i W_k^i,$$

$$Q_k^i = q_k + h\sum_{j=1}^{s} a_{ij} V_k^j, \qquad P_k^i = p_k + h\sum_{j=1}^{s} \hat{a}_{ij} W_k^j,$$

$$W_k^i = D_1 L(Q_k^i, V_k^i) + \left\langle \Lambda_k^i, D_2\Phi(Q_k^i, V_k^i)\right\rangle, \quad P_k^i = D_2 L(Q_k^i, V_k^i),$$

$$q_k^i = Q_k^i, \qquad p_k^i = p_k + h\sum_{j=1}^{s} a_{ij} W_k^j,$$

$$p_k = D_2 L(q_k, v_k), \qquad p_k^i = D_2 L(q_k^i, v_k^i)$$

$$\Phi(q_k^i, v_k^i) = 0$$

Discrete nonholonomic mechanics IV

Key players

$$Q_k^i = q_k + h\sum_{j=1}^{s} a_{ij} V_k^j, \qquad P_k^i = p_k + h\sum_{j=1}^{s} \hat{a}_{ij} W_k^j, \qquad p_k^i = p_k + h\sum_{j=1}^{s} a_{ij} W_k^j$$

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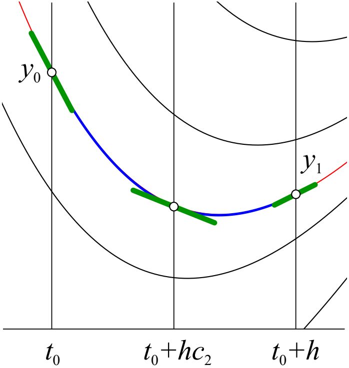

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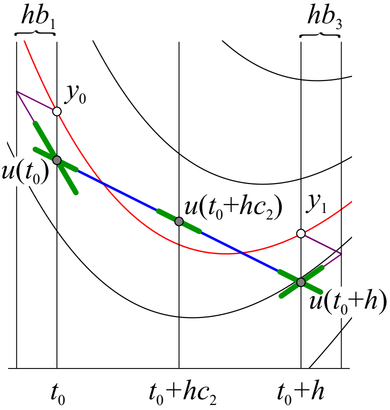

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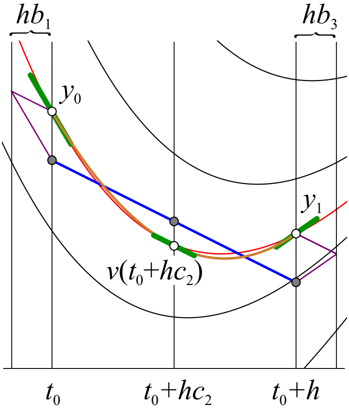
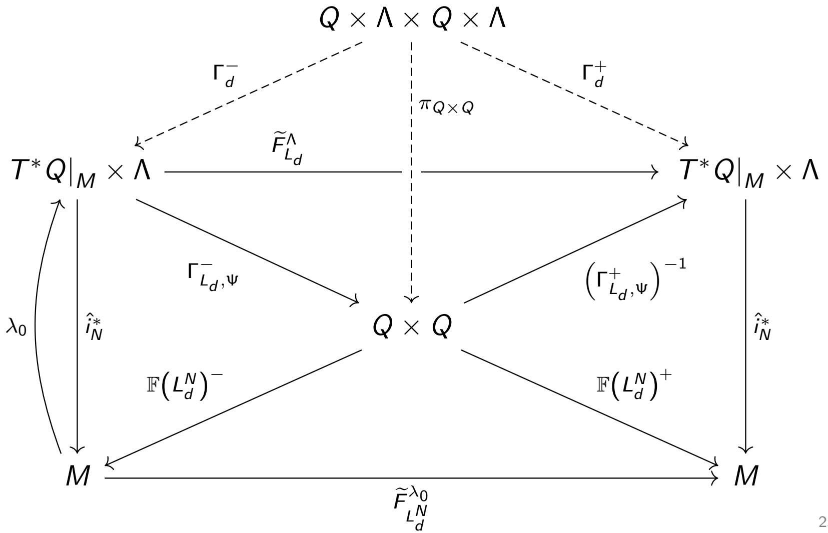


Discrete nonholonomic mechanics V



Discrete nonholonomic mechanics VI

Unfortunately, the variational error theorem does not apply. We need to prove order using numerical analysis techniques.

Theorem. Global error

If we use an s-stage member of the Lobatto-type family [...] the order of the nonholonomic Hamiltonian flow generated by the former integrator is $r = 2s - 2$ in M thus achieving parity with the expected variational error.

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The starting point (again)

Hamilton-Pontryagin action on Lie groups

$(g, v, p) : [a, b] \subset \mathbb{R} \to \mathbb{T}G := TG \oplus T^*G.$

$$\mathcal{J}_{\mathcal{HP}}(g, v, p) = \int_0^h \left[L(g(t), v(t)) + \langle p(t), \dot{g}(t) - v(t) \rangle \right] \mathrm{d}t$$

Dynamical equations

$$\begin{aligned} \frac{\mathrm{d}p(t)}{\mathrm{d}t} &= D_1 L(g(t), v(t)), \\ p(t) &= D_2 L(g(t), v(t)), \\ \frac{\mathrm{d}g(t)}{\mathrm{d}t} &= v(t), \quad \forall t \in [0, h]. \end{aligned}$$

Partially reduced case

Reduced Hamilton-Pontryagin action

$(g, \eta, \mu) : [a, b] \subset \mathbb{R} \to G \times \mathfrak{g} \times \mathfrak{g}^*$, $\ell : G \times \mathfrak{g} \to \mathbb{R}$.

$$\mathcal{J}_{\mathcal{HP}}(g, \eta, \mu) = \int_0^h \left[\ell(g(t), \eta(t)) + \left\langle \mu(t), g^{-1}(t)\dot{g}(t) - \eta(t) \right\rangle \right] \mathrm{d}t$$

Reduced Dynamical equations

$$\begin{aligned} \frac{\mathrm{d}\mu(t)}{\mathrm{d}t} &= \mathrm{ad}^*_{\eta(t)}\mu(t) + \left(L_{g(t)}\right)^* D_1\ell(g(t), \eta(t)), \\ \mu(t) &= D_2 L(g(t), \eta(t)), \\ \frac{\mathrm{d}g(t)}{\mathrm{d}t} &= \left(L_{g(t)}\right)_* \eta(t), \quad \forall t \in [0, h]. \end{aligned}$$

Lie group integrators

Assume $L_{h^{-1}}g \in U_e$ and let $\tau : \mathfrak{g} \to U_e \subset G$ be a retraction.

$$
\begin{array}{ccccc}
\mathbb{T}\mathfrak{g} & \underset{\mathbb{T}\tau^{-1}}{\overset{\mathbb{T}\tau}{\rightleftarrows}} & \mathbb{T}U_e & \underset{\mathbb{T}L_h^{-1}=\mathbb{T}L_{h^{-1}}}{\overset{\mathbb{T}L_h}{\rightleftarrows}} & \mathbb{T}G \\
\downarrow \pi_{\mathfrak{g}} & & \downarrow \pi_U & & \downarrow \pi_G \\
\mathfrak{g} & \underset{\tau^{-1}}{\overset{\tau}{\rightleftarrows}} & U_e & \underset{L_h^{-1}=L_{h^{-1}}}{\overset{L_h}{\rightleftarrows}} & G
\end{array}
$$

$$
\begin{aligned}
(\xi, \eta, \mu) &= \mathbb{T}_{L_{h^{-1}}g}\tau^{-1}\mathbb{T}_g L_{h^{-1}}(g, v_g, p_g) \\
&= \left(\tau^{-1}(L_{h^{-1}}g), \mathrm{d}^L\tau^{-1}_{\tau^{-1}(L_{h^{-1}}g)} T_g L_{g^{-1}} v_g, \left(\mathrm{d}^L\tau_{\tau^{-1}(L_{h^{-1}}g)}\right)^* (T_e L_g)^* p_g\right) \\
(g, v_g, p_g) &= \mathbb{T}_{\tau(\xi)} L_h \mathbb{T}_\xi \tau(\xi, \eta, \mu) \\
&= \left(L_h\tau(\xi), T_e L_{L_h\tau(\xi)} \mathrm{d}^L\tau_\xi \eta, \left(T_{L_h\tau(\xi)} L_{(L_h\tau(\xi))^{-1}}\right)^* \left(\mathrm{d}^L\tau_\xi^{-1}\right)^* \mu_\xi\right)
\end{aligned}
$$

where $\mathrm{d}^L\tau : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ left-trivialized tangent of τ.

Variational Lie group integrators

Reduced discrete Hamilton-Pontryagin action

$\ell : G \times \mathfrak{g} \to \mathbb{R}$ partially reduced Lagrangian.

$$
\begin{aligned}
(\mathcal{J}_{\mathcal{HP}})_d = \sum_{k=0}^{N-1} \sum_{i=1}^{s} h \Bigg[& b_i \ell \left(g_k \tau(\xi_k^i), \mathrm{d}^L \tau_{\xi_k^i} \eta_k^i \right) \\
& + \left\langle \widetilde{M}_k^i, \frac{1}{h} \xi_k^i - \sum_{j=1}^{s} a_{ij} \eta_k^j \right\rangle \\
& + \left\langle \tilde{\mu}_{k+1}, \frac{1}{h} \tau^{-1}((g_k)^{-1} g_{k+1}) - \sum_{j=1}^{s} b_j \eta_k^j \right\rangle \Bigg]
\end{aligned}
$$

Variational Lie group integrators

Discrete dynamical equations

$$
\begin{aligned}
\xi_k^i &= \tau^{-1}\left(g_k^{-1}G_k^i\right) = h\sum_{j=1}^{s} a_{ij}\eta_k^j,\\
\xi_{k,k+1} &= \tau^{-1}\left(g_k^{-1}g_{k+1}\right) = h\sum_{j=1}^{s} b_j\eta_k^j,\\
\mathrm{M}_k^i &= \mathrm{Ad}^*_{\tau(\xi_{k,k+1})}\left[\mu_k + h\sum_{j=1}^{s} b_j\left(\mathrm{d}^L\tau^{-1}_{-\xi_k^j} - \frac{a_{ji}}{b_i}\mathrm{d}^L\tau^{-1}_{-\xi_{k,k+1}}\right)^*\mathrm{N}_k^j\right],\\
\mu_{k+1} &= \mathrm{Ad}^*_{\tau(\xi_{k,k+1})}\left[\mu_k + h\sum_{j=1}^{s} b_j\left(\mathrm{d}^L\tau^{-1}_{-\xi_k^j}\right)^*\mathrm{N}_k^j\right],\\
\mathrm{N}_k^i &= \left(\mathrm{d}^L\tau_{\xi_k^i}\right)^* L^*_{g_k\tau(\xi_k^i)} D_1\ell\left(g_k\tau(\xi_k^i), \mathrm{d}^L\tau_{\xi_k^i}\eta_k^i\right),\\
\mathrm{M}_k^i &= \left(\mathrm{d}^L\tau^{-1}_{\xi_{k,k+1}}\right)^*\left[\Pi_k^i + h\sum_{j=1}^{s}\frac{b_j a_{ji}}{b_i}\left(\mathrm{dd}^L\tau_{\xi_k^j}\right)^*\left(\eta_k^j, \Pi_k^j\right)\right],\\
\Pi_k^i &= \left(\mathrm{d}^L\tau_{\xi_k^i}\right)^* D_2\ell\left(g_k\tau(\xi_k^i), \mathrm{d}^L\tau_{\xi_k^i}\eta_k^i\right),\\
\mu_k &= \left(\mathrm{d}^L\tau^{-1}_{\xi_{k-1,k}}\right)^*\tilde{\mu}_k.
\end{aligned}
$$

Variational Lie group integrators

Second trivialized differential of τ

$\mathrm{dd}^L\tau : \mathfrak{g} \times \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ linear map on second and third arguments s.t.:

$$\partial_\xi \left(\mathrm{d}^L\tau_\xi \eta \right) \delta\xi = \mathrm{d}^L\tau_\xi \mathrm{dd}^L\tau_\xi(\eta, \delta\xi).$$

Appears naturally when considering elements from $T^{(2)}G$ represented by elements $(\xi, \eta, \zeta) \in T^{(2)}\mathfrak{g}$:

$$\left(\tau(\xi), \tau(\xi)\mathrm{d}^L\tau_\xi\eta, \tau(\xi)\mathrm{d}^L\tau_\xi \left[\zeta + \mathrm{dd}^L\tau_\xi \left(\eta, \eta \right) \right] \right)$$

Nonholonomic Lie group integrators

Modified discrete dynamical equations

$$\mathrm{N}_k^i = \left(\mathrm{d}^L\tau_{\xi_k^i}\right)^* \left[L^*_{g_k\tau(\xi_k^i)} D_1\ell\left(g_k\tau(\xi_k^i), \mathrm{d}^L\tau_{\xi_k^i}\eta_k^i\right)\right.$$
$$\left. + \left\langle \Lambda_k^i, D_2\phi\left(g_k\tau(\xi_k^i), \mathrm{d}^L\tau_{\xi_k^i}\eta_k^i\right)\right\rangle\right]$$

$$g_k^i = G_k^i$$

$$\mu_k^i = \mathrm{Ad}^*_{\tau(\xi_k^i)}\left[\mu_k + h\sum_{j=1}^{s} a_{ij}\left(\mathrm{d}^L\tau^{-1}_{-\xi_k^j}\right)^* \mathrm{N}_k^j\right]$$
$$\psi\left(g_k^i, \mu_k^i\right) = 0$$

where $\phi : G \times \mathfrak{g} \to \mathbb{R}$ and $\phi \circ \mathbb{F}\ell^{-1} = \psi : G \times \mathfrak{g}^* \to \mathbb{R}$.

Convergence rates coincide with their vector space counterparts.

THANKS FOR YOUR ATTENTION!