Discrete Dynamics and Variational Integrators

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Introduction

- Discrete dynamics is a complete and self-contained theory of dynamics
- Time is regarded as a discrete variable ab initio
- The scope and structure of the theory is identical to that of Lagrangian and Hamiltonian mechanics
- Time-integrators are a byproduct of the theory
- Discrete dynamics possesses a Noether’s thm
- Variational integrators are symplectic and energy/momentum conserving
- Veselov (1988); Marsden and Wendlandt (1997)
Classical Lagrangian mechanics

- \( Q \equiv \text{Configuration manifold, e.g., } Q = E(n)^N \)
- \( TQ \equiv \text{Tangent bundle} \)
- \( L : TQ \times \mathbb{R} \to \mathbb{R} \equiv \text{Lagrangian} \)
- \( S : Q^{[a,b]} \to \mathbb{R} \equiv \text{Action integral}, \quad S = \int_a^b L(q(t), \dot{q}(t), t) \, dt \)

- **Hamilton’s principle:** \( \delta S = 0, \quad \delta q(a) = \delta q(b) = 0 \)
\textbf{Lagrangian mechanics – Noether’s thm}

- \( G \equiv \text{Lie group}, \ T_eG \equiv \text{Lie algebra} \)

- Left action of \( G \) on \( Q \) is \( \Phi : G \times Q \rightarrow Q \) s. t.
  
  \begin{enumerate}
  \item \( \Phi(e, q) = q, \quad \forall q \in Q \)
  \item \( \Phi(g, \Phi(h, q)) = \Phi(gh, q), \quad \forall q \in Q, \ \forall g, h \in G \)
  \end{enumerate}

- Generator: Given \( \xi \in T_eG, \ \xi_Q \in TQ \) s. t.
  
  \[ \xi_Q(q) = \frac{d}{dt} [\Phi(\exp(t\xi), q)]_{t=0} \]

- \textbf{Momentum map:} \( J : TQ \times \mathbb{R} \rightarrow T^*_eG \) s. t.
  
  \[ \langle J(q, \dot{q}, t), \xi \rangle = \langle p, \xi_Q(q) \rangle, \quad \forall \xi \in T_eG \]
Theorem (Noether’s theorem) Let $Q$ be a smooth manifold and $G$ a Lie group acting on $Q$. Let $L : TQ \times \mathbb{R} \to \mathbb{R}$ be a Lagrangian invariant under $G$. Then the momentum map $J$ is a constant of the motion.

Examples:

i) Linear momentum: $Q = E(n)^N$, $G = E(n)$. 
$\Phi(u, q) = \{q_1 + u, \ldots, q_N + u\} \equiv \text{translations}$. 
Momentum map: $J = \sum_{a=1}^{N} p_a$

ii) Angular momentum: $Q = E(n)^N$, $G = SO(n)$. 
$\Phi(R, q) = \{Rq_1, \ldots, Rq_N\} \equiv \text{rotations}$. 
Momentum map: $J = \sum_{a=1}^{N} q_a \times p_a$
Conservation of energy - Spacetime

- $\mathcal{Q} = \mathbb{R} \times Q \equiv \text{Spacetime configuration manifold}$

- $\mathbb{L}\left((q_0, q), (q'_0, q')\right) = L(q, q'/q'_0, q_0) q'_0$
  $\equiv \text{Spacetime Lagrangian}$

Examples:

iii) \textbf{Energy}: $\mathcal{Q} = \mathbb{R} \times Q, \quad G = \mathbb{R}.$

\[ \Phi(\xi, (q_0, q)) = (q_0 + \xi, q) \equiv \text{time-shift}. \]

Momentum map: $J = L - p \cdot \dot{q} \equiv -E$
Time integration – ODE approach

- Euler-Lagrange (semidiscrete) equations:

\[-\frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i} + \frac{\partial L}{\partial q^i} = 0\]

- Discretize in time as a system of ODEs

- **Example:** $L = (1/2) \dot{q}^T M \dot{q} - V(q, t)$, 

  Newmark algorithm:

  \[
  q_{n+1} = q_n + \Delta t v_n + \Delta t^2 \left[ (1/2 - \beta) a_n + \beta a_{n+1} \right] \\
  v_{n+1} = v_n + \Delta t \left[ (1 - \gamma) a_n + \gamma a_{n+1} \right] \\
  M a_{n+1} + D V(q_{n+1}, t_{n+1}) = 0
  \]

- Variational structure neglected, no Noether’s thm!
Discrete Lagrangian mechanics

- Vesselov (1988), Marsden and Wendlandt (1997)
- $L_d : Q \times Q \rightarrow \mathbb{R} \equiv \text{Discrete Lagrangian,}$
  \[ L_d \approx \int_{t_k}^{t_{k+1}} L(q(t), \dot{q}(t)) \, dt \]
- $S_d : Q^{N+1} \rightarrow \mathbb{R} \equiv \text{Action sum,}$
  \[ S_d = \sum_{k=0}^{N-1} L_d(q_k, q_{k+1}) \]
- Discrete Hamilton’s principle: $\delta S_d = 0,$
  \[ \delta q_0 = \delta q_N = 0 \]
Discrete Lagrangians - Examples

- Restrict \( S \) to piecewise-linear trajectories:
  \[
  L_d = \int_{t_k}^{t_{k+1}} L \left( \frac{t_{k+1} - t}{t_{k+1} - t_k} q_k + \frac{t - t_k}{t_{k+1} - t_k} q_{k+1}, \frac{q_{k+1} - q_k}{t_{k+1} - t_k} \right) dt
  \]

- Generalized midpoint rule (GMR):
  \[
  L_d = (t_{k+1} - t_k) L \left( (1 - \alpha) q_k + \alpha q_{k+1}, \frac{q_{k+1} - q_k}{t_{k+1} - t_k} \right)
  \]

- Generalized trapezoidal rule (GTR):
  \[
  L_d = (t_{k+1} - t_k) \times \left\{ (1 - \alpha) L \left( q_k, \frac{q_{k+1} - q_k}{t_{k+1} - t_k} \right) + \alpha L \left( q_{k+1}, \frac{q_{k+1} - q_k}{t_{k+1} - t_k} \right) \right\}
  \]
Relation to Newmark’s algorithm

- Kane, Marsden, Ortiz and West (2000).

**Theorem** (Shadowing property) Let $L = (1/2) \dot{q}^T M \dot{q} - V(q)$ and let $\{q_k\}$ be a trajectory of the GMR discrete Lagrangian with $\Delta t = \text{constant}$. Then, $\{(1 - \alpha)q_k + \alpha q_{k+1}\}$ satisfies Newmark’s algorithm with $\gamma = 1/2$ and $\beta = \alpha(1 - \alpha)$. 
Variational structure of Newmark

**Theorem.** Let \( L = (1/2) \dot{q}^T M \ddot{q} - V(q) \). Let

\[
\eta(q) = q - \beta \Delta t^2 M^{-1} D V(q)
\]

Then, there exists a function \( \tilde{V} : Q \rightarrow \mathbb{R} \) such that

\[
D \tilde{V}(\eta(q)) = D V(q)
\]

Let \( \gamma = 1/2 \) and \( \Delta t = \text{constant} \). Then, Newmark’s algorithm is variational with discrete Lagrangian

\[
L_d(q_k, q_{k+1}) = \tilde{L}_d(\eta(q_k), \eta(q_{k+1}))
\]

where \( \tilde{L}_d(q_k, q_{k+1}) \) is the GMR discrete Lagrangian for \( \tilde{L} = (1/2) \dot{q}^T M \dot{q} - \tilde{V}(q) \).
Discrete Noether’s theorem

- Discrete Euler-Lagrange equations:
  \[ D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k) = 0 \]

- Discrete Momentum map: \( J_d : Q \times Q \to T^*_e G \) s. t.
  \[ \langle J_d(q_k, q_{k+1}), \xi \rangle = \langle D_2 L_d(q_k, q_{k+1}), \xi_Q(q_{k+1}) \rangle \]

**Theorem** (Discrete Noether’s theorem) Let \( Q \) be a smooth manifold and \( G \) a Lie group acting on \( Q \). Let \( L_d : Q \times Q \to \mathbb{R} \) be a discrete Lagrangian invariant under \( G \). Then the discrete momentum map \( J_d \) is a constant of the discrete motion.
Discrete Noether’s theorem

Examples: \( L = (1/2) \dot{q}^T M \dot{q} - V(q) \), \( L_d \equiv \text{GMR} \)

i) **Linear momentum**: \( Q = E(n)^N \), \( G = E(n) \).
\[ \Phi(u, q) = \{ q_1 + u, \ldots, q_N + u \} \equiv \text{translations}. \]
Discrete momentum map:
\[
J_d = \sum_{a=1}^{N} m_a \frac{q_{a}^{k+1} - q_{a}^{k}}{t_{k+1} - t_{k}}
\]

ii) **Angular momentum**: \( Q = E(n)^N \), \( G = SO(n) \).
\[ \Phi(R, q) = \{ Rq_1, \ldots, Rq_N \} \equiv \text{rotations}. \]
Discrete momentum map:
\[
J_d = \sum_{a=1}^{N} q_{a}^{k+1} \times \left( m_a \frac{q_{a}^{k+1} - q_{a}^{k}}{t_{k+1} - t_{k}} \right)
\]
Global energy conservation - Spacetime

- Kane, Marsden and Ortiz (1999)

iii) **Energy**: \( \mathbb{Q} = \mathbb{R} \times \mathbb{Q}, \quad G = \mathbb{R} \).

\[
\mathbb{L}\left((q_0, q), (q'_0, q')\right) = L(q, q'/q'_0, q_0) q'_0
\]

\[
\Phi\left(\xi, (q_0, q)\right) = (q_0 + \xi, q) \equiv \text{time shift.}
\]

Discrete momentum map:

\[
J_d = \frac{\partial \mathbb{L}_d}{\partial t_{k+1}} \left((t_k, q_k), (t_{k+1}, q_{k+1})\right) \equiv -E_d
\]

\[
L = \frac{1}{2} \dot{q}^T M \dot{q} - V(q), \quad \mathbb{L}_d \equiv \text{GMR}:
\]

\[
E_d = \frac{1}{2} \left(\frac{q_{k+1} - q_k}{t_{k+1} - t_k}\right)^T M \left(\frac{q_{k+1} - q_k}{t_{k+1} - t_k}\right) + V(q_{k+ \alpha})
\]
Spacetime – Time adaption

- **Spacetime**: $Q = \mathbb{R} \times Q$, $L((q_0, q), (q'_0, q')) = L(q, q'/q'_0, q_0) q'_0$

- Additional discrete Euler-Lagrange equation: $0 = \frac{\partial L_d}{\partial t_k}((t_k, q_k), (t_{k+1}, q_{k+1})) + \frac{\partial L_d}{\partial t_{k+1}}((t_{k+1}, q_{k+1}), (t_k, q_k))$

- Conservation of energy furnishes additional equation which determines $t_{k+1} \Rightarrow \text{Time adaption}$

- Conversely, energy conservation requires time adaption (Ge and Marsden, 1988)
Spacetime - Time adaption

- Kane, Marsden and Ortiz (1999)
- **Example**: GMR, coupled two-well and harmonic potentials:

\[
L\left((x, y), (\dot{x}, \dot{y})\right) = L^{\text{DW}}(x, \dot{x}) + L^{\text{HO}}(y, \dot{y}) + \epsilon xy
\]

![Graphs and phase portraits](image-url)
Asynchronous Variational integrators

- Lew, Marsden, Ortiz and West (2002)
- Assume decomposition into subsystems:

\[ L(q, \dot{q}, t) = \sum_{K \in \mathcal{T}} L_K(q_K, \dot{q}_K, t) \]

where:
- i) \( q_K \in Q_K \equiv \) submanifold of \( Q \)
- ii) \( L_K : TQ_K \times \mathbb{R} \to \mathbb{R} \).

- Endow each subsystem with its own clock:

\[ L_d = \sum_{K \in \mathcal{T}} L^K_d \left( (t^K_d, q^K_d), (t^{K+1}_d, q^{K+1}_d) \right) \]

- Subcycling: T. Belytschko, T. J. R. Hughes, W. K. Liu, P. Smolinski...
AVIs – Local energy balance

- Local Energy:

\[ J^K_d = \frac{\partial \Pi^K_d}{\partial t^K_{k+1}} \left( (t^K_k, q^K_k), (t^K_{k+1}, q^K_{k+1}) \right) \equiv -E^K_d \]

- Local energy balance:

\[ E^K_d \left( (t^K_k, q^K_k), (t^K_{k+1}, q^K_{k+1}) \right) = E^K_d \left( (t^K_{k-1}, q^K_{k-1}), (t^K_k, q^K_k) \right) \]

- Local energy balance equation furnishes additional discrete Euler-Lagrange equation for \( t^{k+1}_K \)

- Alternatively, set \( \Delta t^K_K \) based on Courant (stability) condition
AVIs - Example

(1) 

(2) 

(3) 

(4) 

(5) 

(6)
Apache AH-64 Helicopter
Apache AH-64 Helicopter

- $\omega = 40$ rad/s
- 10-node tets, *slivers*
- AVI, trapeziodal rule
- Element time step: Courant condition

$$\frac{\omega L^2}{c_s \omega} = 1.96, \ 3.08, \ 12.3$$
Apache AH-64 Helicopter

- Max/Min # of calls/element = $235 \times 10^6 / 12 \times 10^6$
- Total # of element calls:
  - AVI: $85 \times 10^9$
  - Newmark: $490 \times 10^9$

\[
\text{Speed-up} = 5.8
\]
Apache AH-64 Helicopter

STABLE CASE

\[ \omega L^2/c_s w = 1.96 \]

UNSTABLE CASE - I

\[ \omega L^2/c_s w = 3.08 \]

UNSTABLE CASE - II

\[ \omega L^2/c_s w = 12.3 \]

AVI calculations, global and local energy histories

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Concluding remarks

- VIs are **symplectic** (Wendlandt and Marsden, 1997; Marsden, Patrick and Shkoller, 1998)

- **Convergence** of VIs and AVIs has been established by forward error analysis (Marsden and West, 2001; Lew and West, in preparation)

- Extensions to **dissipative systems** are possible (Kane, Marsden, Ortiz and West, 2000)

- VIs and AVIs can be extended to PDE’s using **multisymplectic geometry** (Marsden, Patrick and Shkoller, 1998; Reich and Bridges, 1999; Lew, Marsden, Ortiz and West, 2002)
Concluding remarks (cont’d)

- Energy-momentum-preserving **contact algorithms** (Fetecau, Marsden, Ortiz and West, 2002)
- Applications to fluids, molecular dynamics, shock physics, general relativity, in progress...