

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)

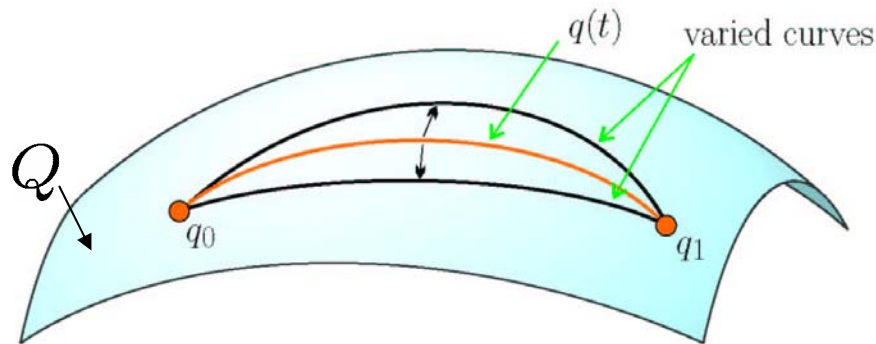


Classical Lagrangian mechanics

- $Q \equiv$ Configuration manifold, e. g., $Q = E(n)^N$
- $TQ \equiv$ Tangent bundle
- $L : TQ \times \mathbb{R} \rightarrow \mathbb{R} \equiv$ Lagrangian
- $S : Q^{[a,b]} \rightarrow \mathbb{R} \equiv$ Action integral,

$$S = \int_a^b L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t) dt$$

- **Hamilton's principle:** $\delta S = 0$, $\delta \mathbf{q}(a) = \delta \mathbf{q}(b) = 0$



Lagrangian mechanics – Noether's thm

- $G \equiv$ Lie group, $T_e G \equiv$ Lie algebra
- Left action of G on Q is $\Phi : G \times Q \rightarrow Q$ s. t.
 - i) $\Phi(e, q) = q, \quad \forall q \in Q$
 - ii) $\Phi(g, \Phi(h, q)) = \Phi(gh, q), \quad \forall q \in Q, \quad \forall g, h \in G$

- Generator: Given $\xi \in T_e G, \quad \xi_Q \in TQ$ s. t.

$$\xi_Q(q) = \frac{d}{dt} [\Phi(\exp(t\xi), q)]_{t=0}$$

- **Momentum map:** $J : TQ \times \mathbb{R} \rightarrow T_e^* G$ s. t.

$$\langle J(q, \dot{q}, t), \xi \rangle = \langle p, \xi_Q(q) \rangle, \quad \forall \xi \in T_e G$$



Lagrangian mechanics – Noether's thm

Theorem (Noether's theorem) *Let Q be a smooth manifold and G a Lie group acting on Q . Let $L : TQ \times \mathbb{R} \rightarrow \mathbb{R}$ be a Lagrangian invariant under G . Then the momentum map J is a constant of the motion.*

Examples:

i) Linear momentum: $Q = E(n)^N$, $G = E(n)$.

$\Phi(u, q) = \{q_1 + u, \dots, q_N + u\} \equiv$ translations.

Momentum map: $J = \sum_{a=1}^N p_a$

ii) Angular momentum: $Q = E(n)^N$, $G = SO(n)$

$\Phi(R, q) = \{Rq_1, \dots, Rq_N\} \equiv$ rotations.

Momentum map: $J = \sum_{a=1}^N q_a \times p_a$



Conservation of energy - Spacetime

- $\mathbb{Q} = \mathbb{R} \times Q \equiv$ Spacetime configuration manifold
- $\mathbb{L}\left((q_0, \mathbf{q}), (q'_0, \mathbf{q}')\right) = L(\mathbf{q}, \mathbf{q}'/q'_0, q_0) q'_0$
 $\equiv$ Spacetime Lagrangian

Examples:

- iii) *Energy*: $\mathbb{Q} = \mathbb{R} \times Q$, $G = \mathbb{R}$.
 $\Phi(\xi, (q_0, \mathbf{q})) = (q_0 + \xi, \mathbf{q}) \equiv$ time-shift.
Momentum map: $J = L - \mathbf{p} \cdot \dot{\mathbf{q}} \equiv -E$



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

$$\mathbf{q}_{n+1} = \mathbf{q}_n + \Delta t \mathbf{v}_n + \Delta t^2 [(1/2 - \beta) \mathbf{a}_n + \beta \mathbf{a}_{n+1}]$$

$$\mathbf{v}_{n+1} = \mathbf{v}_n + \Delta t [(1 - \gamma) \mathbf{a}_n + \gamma \mathbf{a}_{n+1}]$$

$$\mathbf{M} \mathbf{a}_{n+1} + DV(\mathbf{q}_{n+1}, t_{n+1}) = 0$$

- Variational structure neglected, no Noether's thm!



Discrete Lagrangian mechanics

- Vesselov (1988), Marsden and Wendlandt (1997)

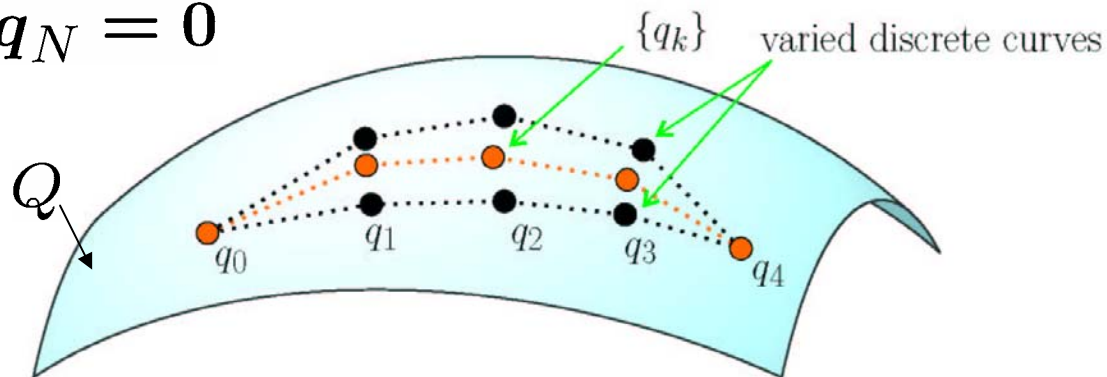
- $L_d : Q \times Q \rightarrow \mathbb{R} \equiv$ Discrete Lagrangian,

$$L_d \approx \int_{t_k}^{t_{k+1}} L(\mathbf{q}(t), \dot{\mathbf{q}}(t)) dt$$

- $S_d : Q^{N+1} \rightarrow \mathbb{R} \equiv$ Action sum, $S_d = \sum_{k=0}^{N-1} L_d(\mathbf{q}_k, \mathbf{q}_{k+1})$

- **Discrete Hamilton's principle:** $\delta S_d = 0,$

$$\delta \mathbf{q}_0 = \delta \mathbf{q}_N = 0$$



Discrete Lagrangians - Examples

- Restrict S to piecewise-linear trajectories: $L_d =$

$$\int_{t_k}^{t_{k+1}} L \left(\frac{t_{k+1} - t}{t_{k+1} - t_k} \mathbf{q}_k + \frac{t - t_k}{t_{k+1} - t_k} \mathbf{q}_{k+1}, \frac{\mathbf{q}_{k+1} - \mathbf{q}_k}{t_{k+1} - t_k} \right) dt$$

- Generalized midpoint rule (GMR):

$$L_d = (t_{k+1} - t_k) L \left((1 - \alpha) \mathbf{q}_k + \alpha \mathbf{q}_{k+1}, \frac{\mathbf{q}_{k+1} - \mathbf{q}_k}{t_{k+1} - t_k} \right)$$

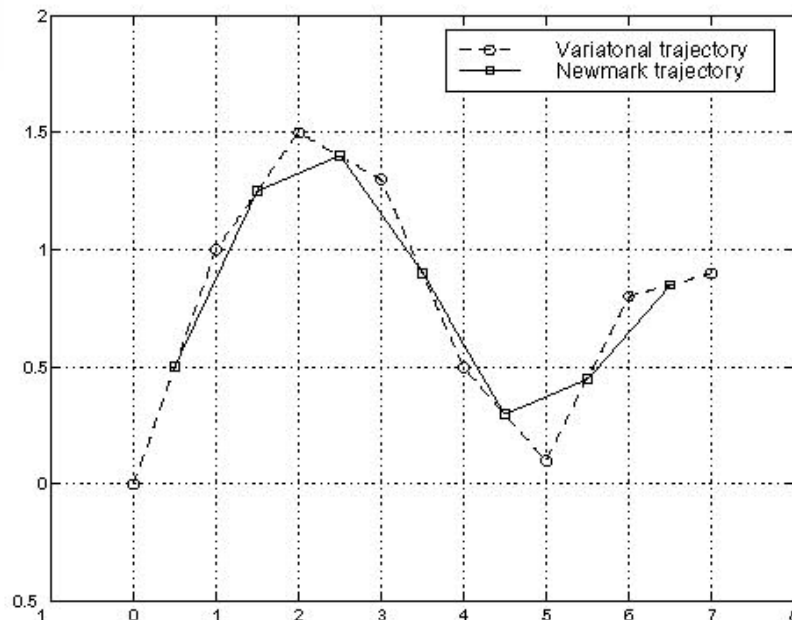
- Generalized trapezoidal rule (GTR): $L_d = (t_{k+1} - t_k) \times \left\{ (1 - \alpha) L \left(\mathbf{q}_k, \frac{\mathbf{q}_{k+1} - \mathbf{q}_k}{t_{k+1} - t_k} \right) + \alpha L \left(\mathbf{q}_{k+1}, \frac{\mathbf{q}_{k+1} - \mathbf{q}_k}{t_{k+1} - t_k} \right) \right\}$



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

$$\eta(q) = q - \beta \Delta t^2 M^{-1} DV(q)$$

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

$$D\tilde{V}(\eta(q)) = DV(q)$$

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:

$$D_1 L_d(\mathbf{q}_k, \mathbf{q}_{k+1}) + D_2 L_d(\mathbf{q}_{k-1}, \mathbf{q}_k) = 0$$

- **Discrete Momentum map:** $J_d : Q \times Q \rightarrow T_e^* G$ s. t.

$$\langle J_d(\mathbf{q}_k, \mathbf{q}_{k+1}), \xi \rangle = \langle D_2 L_d(\mathbf{q}_k, \mathbf{q}_{k+1}), \xi_Q(\mathbf{q}_{k+1}) \rangle$$

Theorem (Discrete Noether's theorem) *Let Q be a smooth manifold and G a Lie group acting on Q . Let $L_d : Q \times Q \rightarrow \mathbb{R}$ 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: $L = (1/2)\dot{\mathbf{q}}^T \mathbf{M} \dot{\mathbf{q}} - V(\mathbf{q})$, $L_d \equiv \text{GMR}$

i) Linear momentum: $Q = E(n)^N$, $G = E(n)$.

$\Phi(\mathbf{u}, \mathbf{q}) = \{\mathbf{q}_1 + \mathbf{u}, \dots, \mathbf{q}_N + \mathbf{u}\} \equiv \text{translations.}$

Discrete momentum map:

$$\mathbf{J}_d = \sum_{a=1}^N m_a \frac{\mathbf{q}_a^{k+1} - \mathbf{q}_a^k}{t_{k+1} - t_k}$$

ii) Angular momentum: $Q = E(n)^N$, $G = SO(n)$

$\Phi(\mathbf{R}, \mathbf{q}) = \{\mathbf{R}\mathbf{q}_1, \dots, \mathbf{R}\mathbf{q}_N\} \equiv \text{rotations.}$

Discrete momentum map:

$$\mathbf{J}_d = \sum_{a=1}^N \mathbf{q}_a^{k+1} \times \left(m_a \frac{\mathbf{q}_a^{k+1} - \mathbf{q}_a^k}{t_{k+1} - t_k} \right)$$



Global energy conservation - Spacetime

- Kane, Marsden and Ortiz (1999)

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

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

$$\Phi(\xi, (q_0, \mathbf{q})) = (q_0 + \xi, \mathbf{q}) \equiv \text{time shift.}$$

Discrete momentum map:

$$J_d = \frac{\partial \mathbb{L}_d}{\partial t_{k+1}}\left((t_k, \mathbf{q}_k), (t_{k+1}, \mathbf{q}_{k+1})\right) \equiv -E_d$$

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

$$E_d = \frac{1}{2} \left(\frac{\mathbf{q}_{k+1} - \mathbf{q}_k}{t_{k+1} - t_k} \right)^T \mathbf{M} \left(\frac{\mathbf{q}_{k+1} - \mathbf{q}_k}{t_{k+1} - t_k} \right) + V(\mathbf{q}_{k+\alpha})$$



Spacetime – Time adaption

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

- Additional discrete Euler-Lagrange equation: $0 =$

$$\frac{\partial \mathbb{L}_d}{\partial t_k} \left((t_k, \mathbf{q}_k), (t_{k+1}, \mathbf{q}_{k+1}) \right) + \frac{\partial \mathbb{L}_d}{\partial t_k} \left((t_{k-1}, \mathbf{q}_{k-1}), (t_k, \mathbf{q}_k) \right)$$

$$E_d \left((t_k, \mathbf{q}_k), (t_{k+1}, \mathbf{q}_{k+1}) \right) = E_d \left((t_{k-1}, \mathbf{q}_{k-1}), (t_k, \mathbf{q}_k) \right)$$

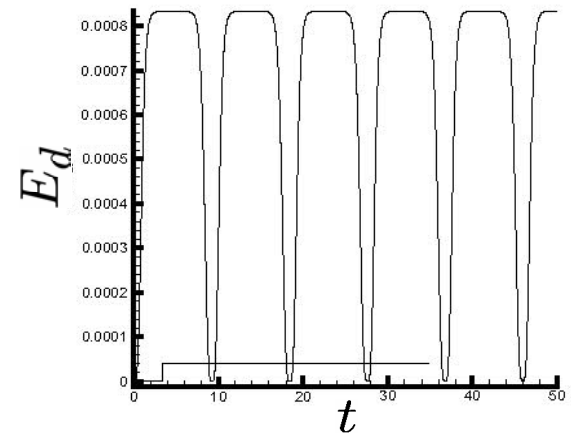
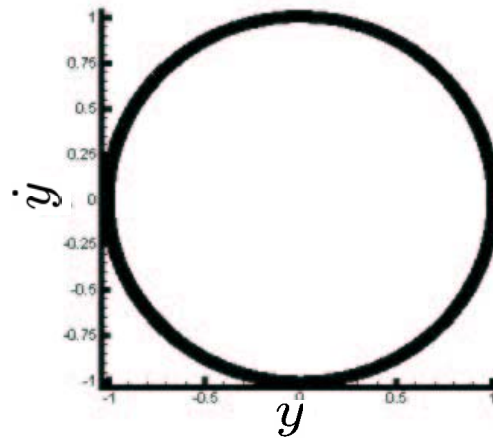
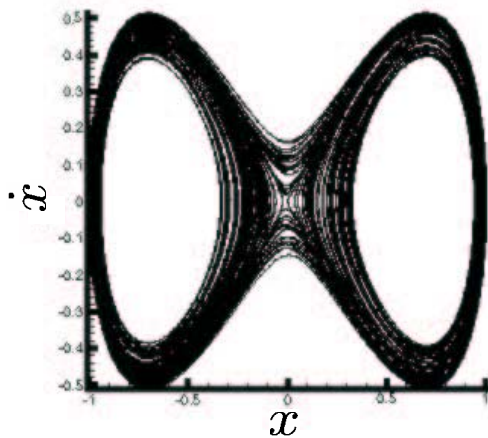
- Conservation of energy furnishes additional equation which determines $t_{k+1} \Rightarrow$ Time adaption
- Conversely, energy conservation requires time adaption (Ge and Marsden, 1988)



Spacetime - Time adaption

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

$$L((x, y), (\dot{x}, \dot{y})) = L^{\text{DW}}(x, \dot{x}) + L^{\text{HO}}(y, \dot{y}) + \epsilon xy$$



Asynchronous Variational integrators

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

$$L(\mathbf{q}, \dot{\mathbf{q}}, t) = \sum_{K \in \mathcal{T}} L_K(\mathbf{q}_K, \dot{\mathbf{q}}_K, t)$$

- where: i) $\mathbf{q}_K \in Q_K \equiv$ submanifold of Q
ii) $L_K : TQ_K \times \mathbb{R} \rightarrow \mathbb{R}$.

- Endow each subsystem with its own *clock*:

$$\mathbb{L}_d = \sum_{K \in \mathcal{T}} \mathbb{L}_d^K \left((t_K^k, \mathbf{q}_K^k), (t_K^{k+1}, \mathbf{q}_K^{k+1}) \right)$$

- Subcycling: T. Belytschko, T. J. R. Hughes, W. K. Liu, P. Smolinski. . .



AVIs – Local energy balance

- *Local Energy:*

$$J_d^K = \frac{\partial \mathbb{L}_d^K}{\partial t_{k+1}^K} \left((t_k^K, \mathbf{q}_k^K), (t_{k+1}^K, \mathbf{q}_{k+1}^K) \right) \equiv -E_d^K$$

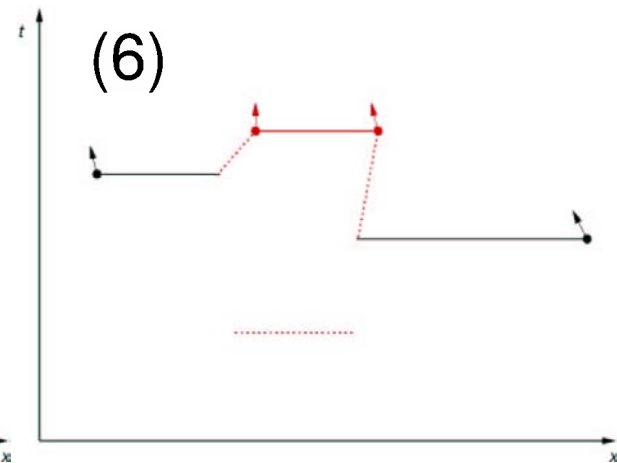
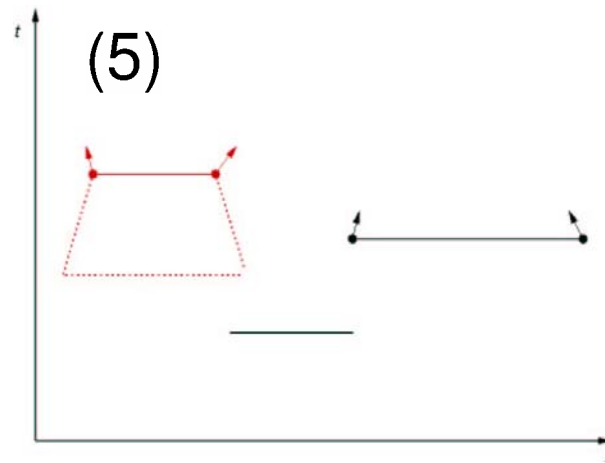
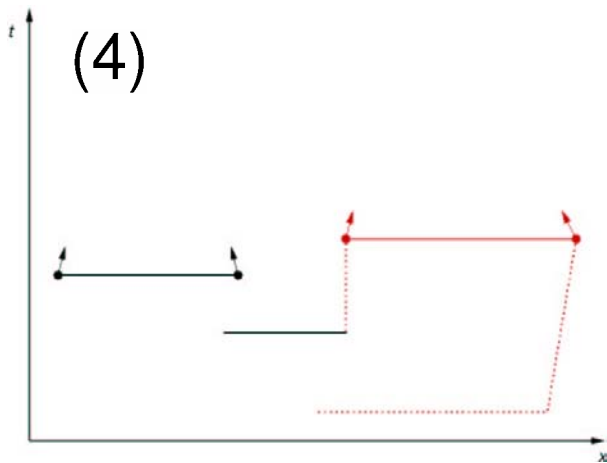
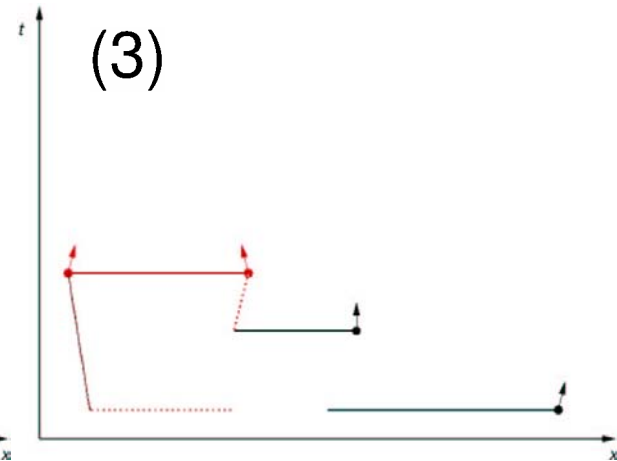
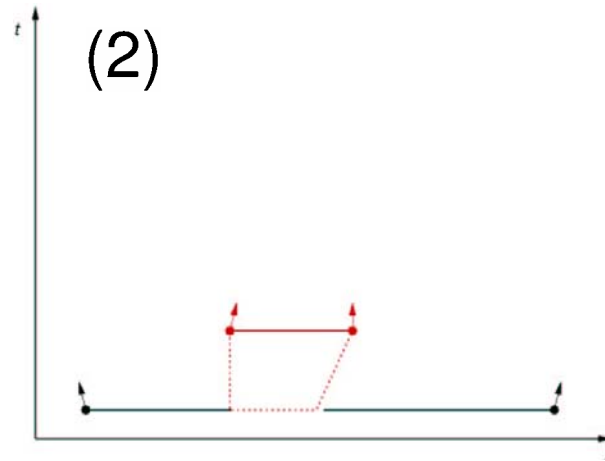
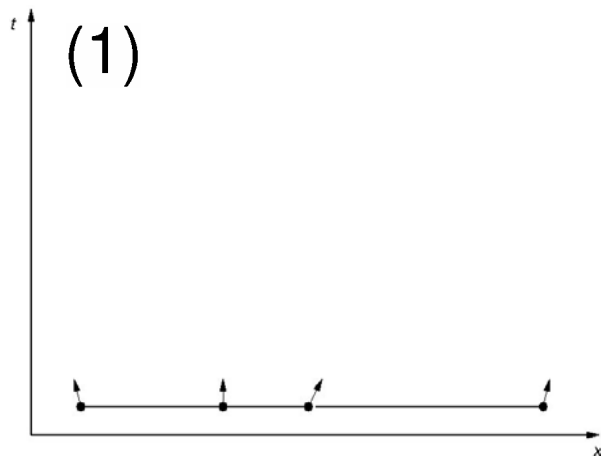
- *Local energy balance:*

$$E_d^K \left((t_k^K, \mathbf{q}_k^K), (t_{k+1}^K, \mathbf{q}_{k+1}^K) \right) = E_d^K \left((t_{k-1}^K, \mathbf{q}_{k-1}^K), (t_k^K, \mathbf{q}_k^K) \right)$$

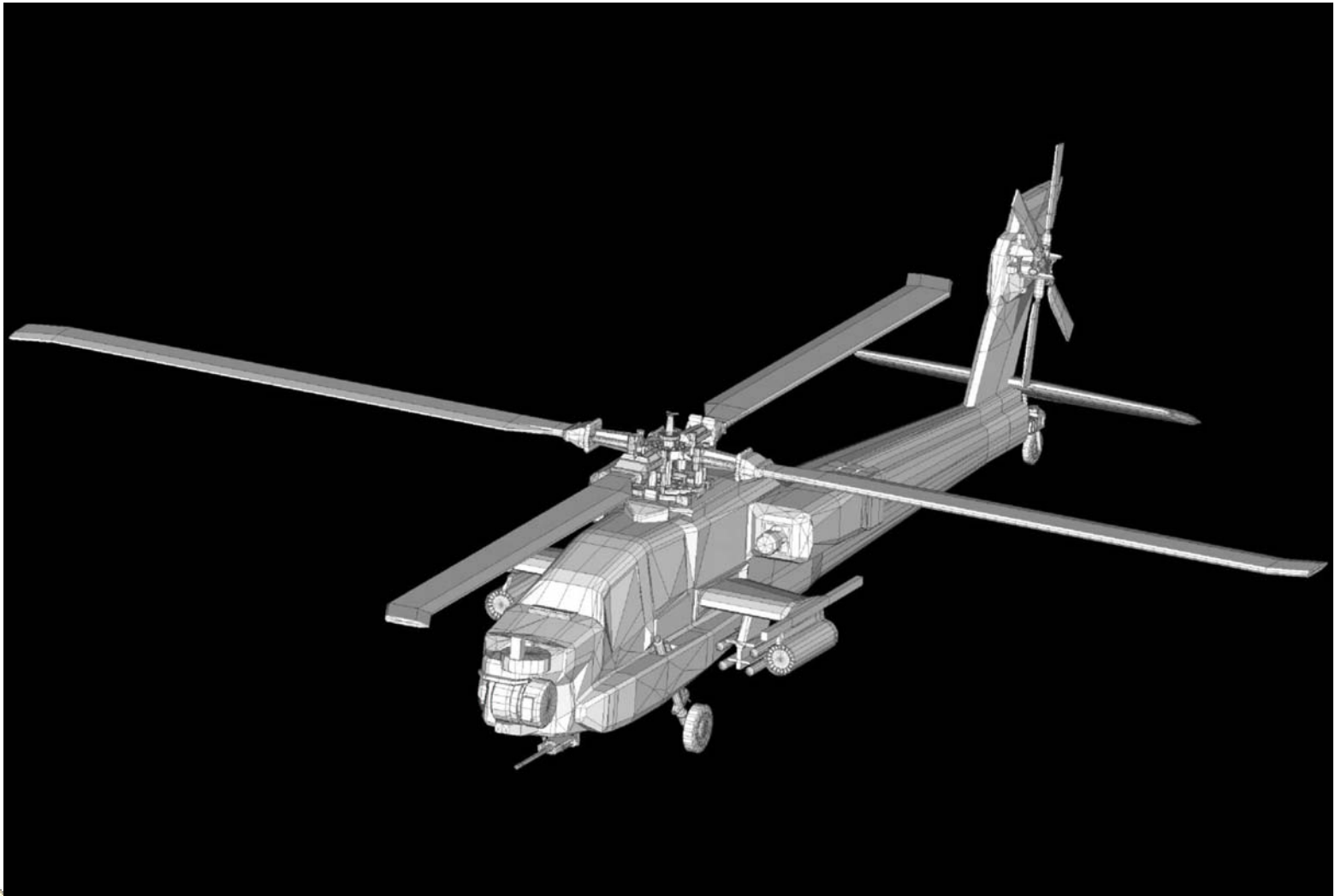
- Local energy balance equation furnishes additional discrete Euler-Lagrange equation for t_K^{k+1}
- Alternatively, set Δt_K based on Courant (stability) condition



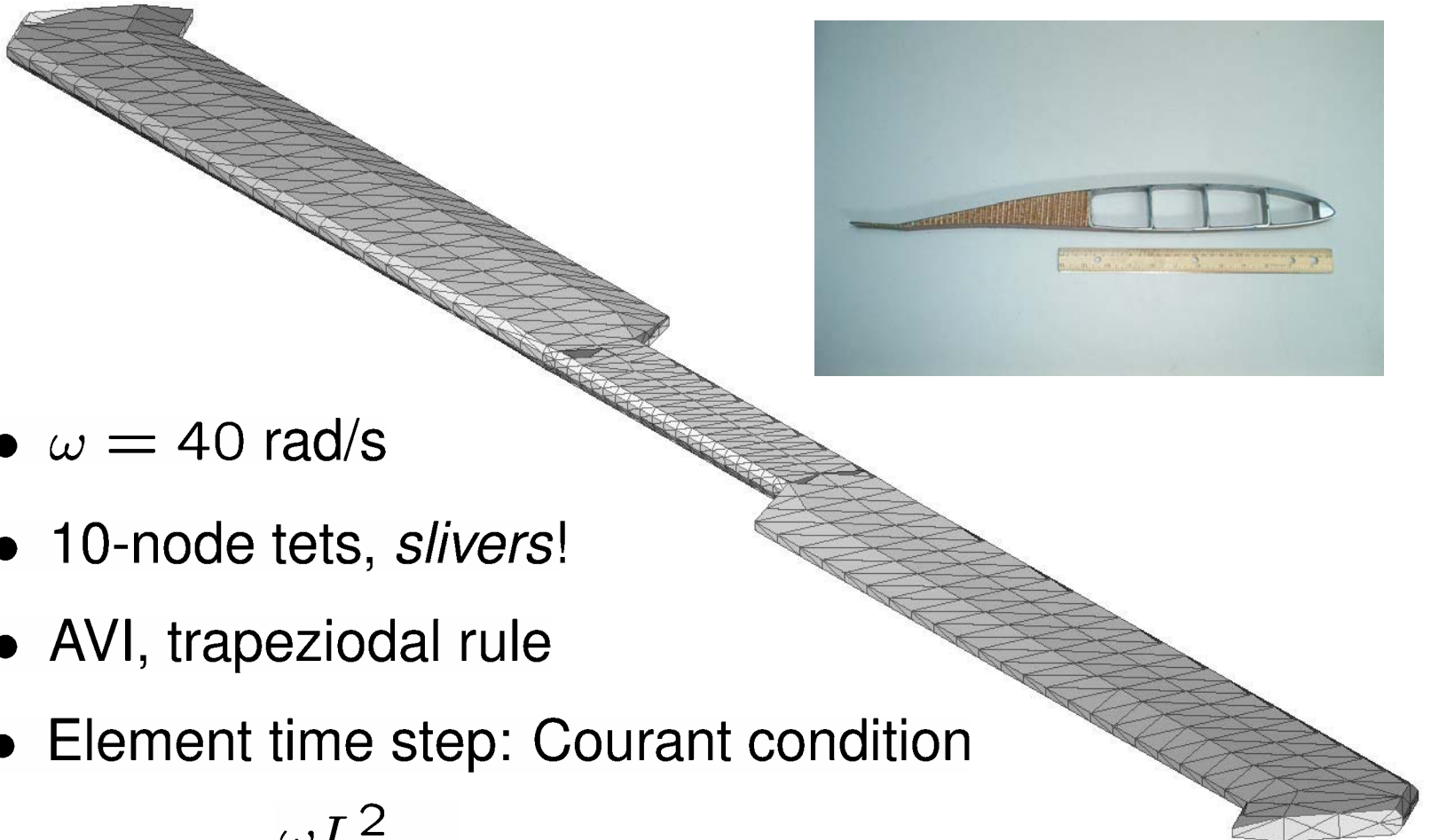
AVIs - Example



Apache AH-64 Helicopter



Apache AH-64 Helicopter

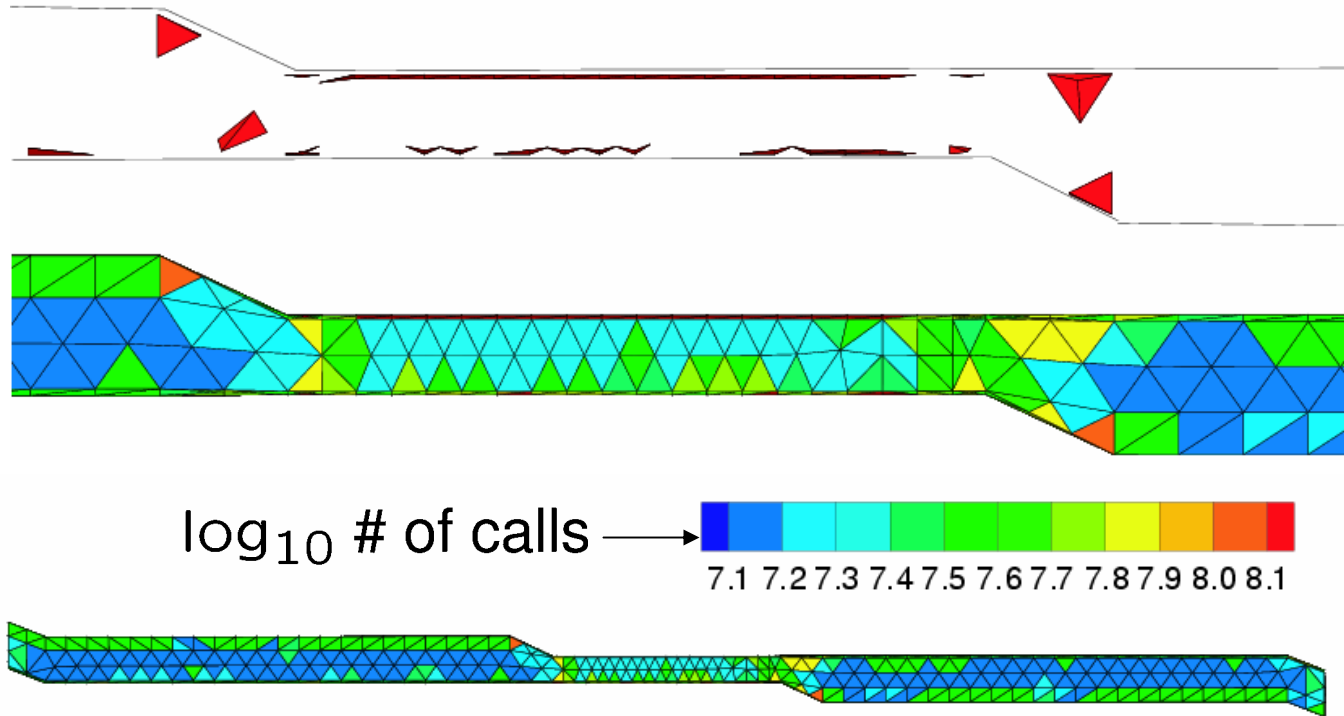


- $\omega = 40 \text{ rad/s}$
- 10-node tets, *slivers*!
- AVI, trapeziodal rule
- Element time step: Courant condition

$$\frac{\omega L^2}{c_s w} = \underline{1.96}, \underline{3.08}, \underline{12.3}$$



Apache AH-64 Helicopter



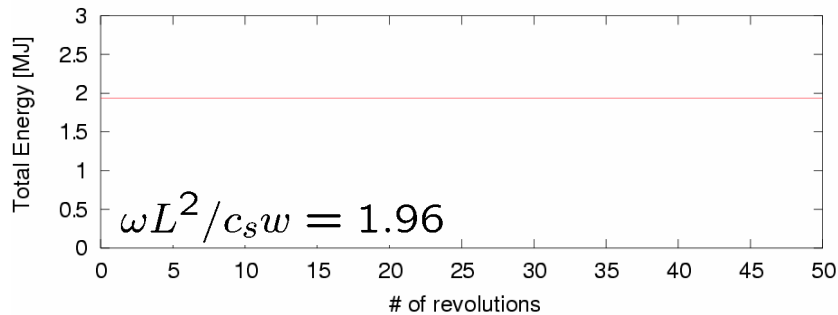
- Max/Min # of calls/element = $235 \times 10^6 / 12 \times 10^6$
- Total # of element calls:
 - AVI: 85×10^9
 - Newmark: 490×10^9

Speed-up = 5.8

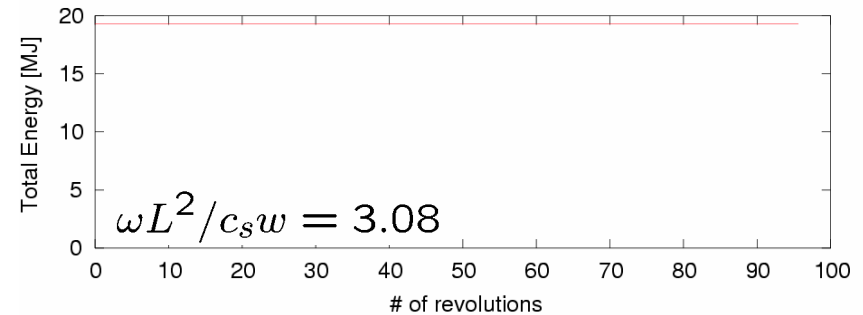


Apache AH-64 Helicopter

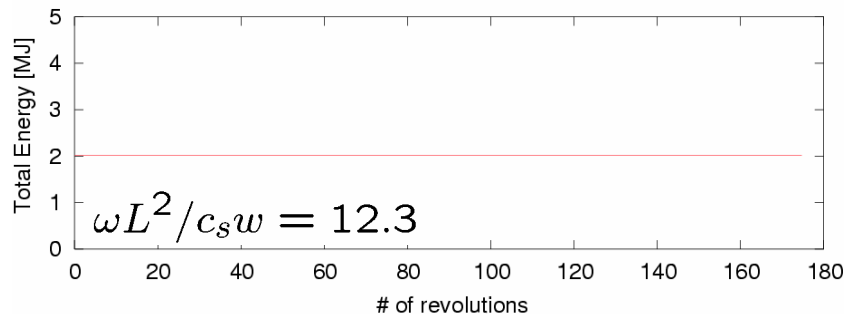
STABLE CASE



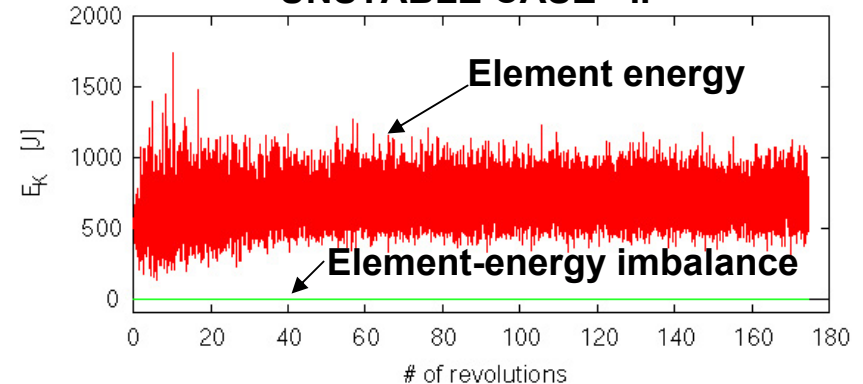
UNSTABLE CASE - I



UNSTABLE CASE - II



UNSTABLE CASE - II



AVI calculations, global and local energy histories



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. . .

