Energy-stepping integrators in Lagrangian mechanics

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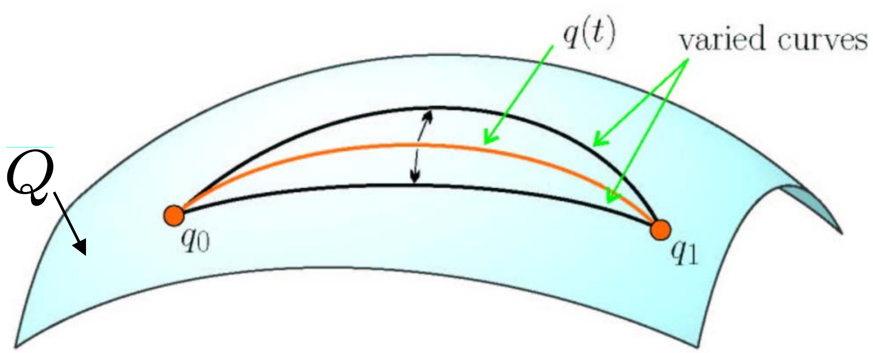
Classical Lagrangian mechanics

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

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

- Hamilton's principle: $\delta S = 0, \qquad \delta q(a) = \delta q(b) = 0$



Hamiltonian picture

- Phase space: $P = T^*Q$
- Hamiltonian: $H(\boldsymbol{q}, \boldsymbol{p}) = \text{sup}_{\boldsymbol{v} \in T_{\boldsymbol{q}}Q} \{\boldsymbol{p} \cdot \boldsymbol{v} - L(\boldsymbol{q}, \boldsymbol{v})\}$
- Canonical symplectic two-form:

$$\Omega = d\boldsymbol{q}_1 \wedge d\boldsymbol{p}_1 + \cdots + d\boldsymbol{q}_N \wedge d\boldsymbol{p}_N$$

- Symplectic manifold: (P, Ω)
- Propagator: $\boldsymbol{z}(t) = (\boldsymbol{q}(t), \boldsymbol{p}(t)) = \varphi_t(\boldsymbol{z}_0)$
- Symplecticity: $\varphi_{t*}\Omega = \Omega$, or

$$\Omega(T\varphi(\boldsymbol{z})\eta_1, T\varphi(\boldsymbol{z})\eta_2) = \Omega(\eta_1, \eta_2)$$

Lagrangian mechanics – Noether's thm

- $G \equiv$ Lie group, $T_eG \equiv$ Lie algebra
- Left action of G on Q is $\Phi : G \times Q \to Q$ s. t.

  i) $\Phi(e, \boldsymbol{q}) = \boldsymbol{q}, \quad \forall \boldsymbol{q} \in Q$

  ii) $\Phi\big(g, \Phi(h, \boldsymbol{q})\big) = \Phi(gh, \boldsymbol{q}), \ \forall \boldsymbol{q} \in Q, \ \forall g, h \in G$

- Generator: Given $\xi \in T_eG$, $\xi_Q \in TQ$ s. t.

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

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

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

Lagrangian mechanics – Noether's thm

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

Examples:

i) *Linear momentum*: $Q = E(n)^N, \quad G = E(n)$.
$\Phi(\boldsymbol{u}, \boldsymbol{q}) = \{\boldsymbol{q}_1 + \boldsymbol{u}, \dots, \boldsymbol{q}_N + \boldsymbol{u}\} \equiv$ translations.
Momentum map: $\boldsymbol{J} = \sum_{a=1}^N \boldsymbol{p}_a$

ii) *Angular momentum*: $Q = E(n)^N, \quad G = SO(n)$
$\Phi(\boldsymbol{R}, \boldsymbol{q}) = \{\boldsymbol{R}\boldsymbol{q}_1, \dots, \boldsymbol{R}\boldsymbol{q}_N\} \equiv$ rotations.
Momentum map: $\boldsymbol{J} = \sum_{a=1}^N \boldsymbol{q}_a \times \boldsymbol{p}_a$

Conservation of energy - Spacetime

- $\mathbb{Q} = \mathbb{R} \times Q \equiv$ Spacetime configuration manifold
- $\mathbb{L}\Big((q_0, \boldsymbol{q}), (q_0', \boldsymbol{q}')\Big) = L(\boldsymbol{q}, \boldsymbol{q}'/q_0', q_0)\, q_0'$
  $\equiv$ Spacetime Lagrangian

Examples:

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

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

$$\boldsymbol{q}_{n+1} = \boldsymbol{q}_n + \triangle t \boldsymbol{v}_n + \triangle t^2 [(1/2 - \beta)\boldsymbol{a}_n + \beta \boldsymbol{a}_{n+1}]$$
$$\boldsymbol{v}_{n+1} = \boldsymbol{v}_n + \triangle t\, [(1 - \gamma)\boldsymbol{a}_n + \gamma \boldsymbol{a}_{n+1}]$$
$$\boldsymbol{M}\boldsymbol{a}_{n+1} + DV(\boldsymbol{q}_{n+1}, t_{n+1}) = \boldsymbol{0}$$

- *Variational structure neglected, no Noether's thm!*

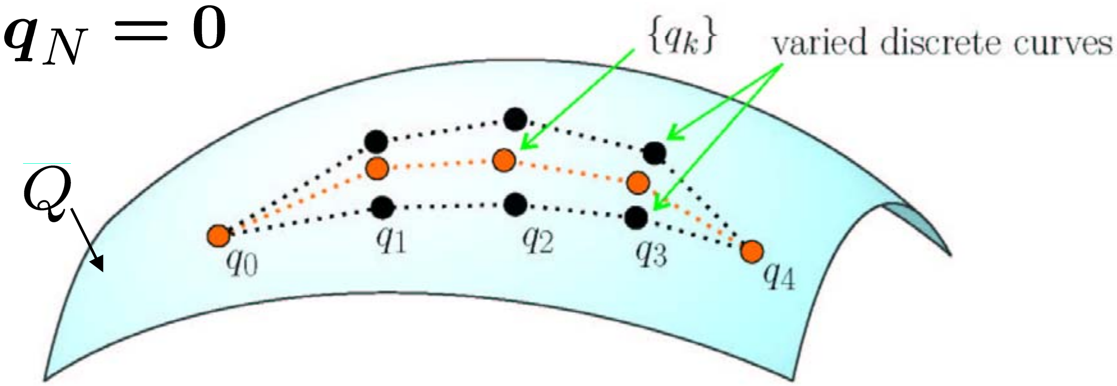
Discrete Lagrangian mechanics

- Vesselov (1988), Marsden and Wendlandt (1997)
- $L_d : Q \times Q \to \mathbb{R} \equiv$ Discrete Lagrangian,

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

- $S_d : Q^{N+1} \to \mathbb{R} \equiv$ Action sum, $S_d = \sum_{k=0}^{N-1} L_d(\boldsymbol{q}_k, \boldsymbol{q}_{k+1})$
- **Discrete Hamilton's principle**: $\boxed{\delta S_d = 0,}$

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



Discrete Noether's theorem

- Discrete Euler-Lagrange equations:

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

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

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

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

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

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

Discrete momentum map:

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

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

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

Discrete momentum map:

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

Discrete Noether's theorem

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

$\mathbb{L}\Big((q_0, \boldsymbol{q}), (q_0', \boldsymbol{q}')\Big) = L(\boldsymbol{q}, \boldsymbol{q}'/q_0', q_0)\, q_0'$

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

Discrete momentum map:

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

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

- Energy eq. determines $t_{k+1} \Rightarrow$ *Time adaption*
- Conversely: Energy conservation requires time adaption (Ge and Marsden, 1988)

Discrete Symplecticity

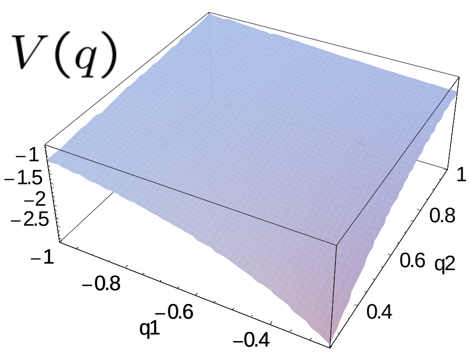
- Discrete momentum: $\boldsymbol{p}_k = -D_1 L_d(\boldsymbol{q}_k, \boldsymbol{q}_{k+1})$
- Discrete propagator: $(\boldsymbol{q}_{k+1}, \boldsymbol{p}_{k+1}) = \varphi_{\Delta t}(\boldsymbol{q}_k, \boldsymbol{p}_k)$
- Discrete symplecticity: $\varphi_{\Delta t *}\Omega = \Omega$
- Variational integrators are symplectic methods in the standard sense!

Variational integrators – Appraisal

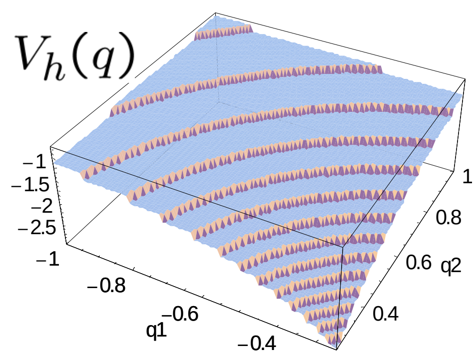
- Variational integrators are symplectic
- Discrete trajectories conserve *discrete* momentum maps exactly
- Discrete momentum maps approximate (but differ from) time-continuous momentum maps
- Ambiguity in choice of discrete Lagrangian
- No guarantee of solvability of the discrete Euler-Lagrange equations (e.g., energy equation)
- Variational structure is no guarantee of convergence of the discrete trajectory
- Some schemes of interest may not be variational (e.g., absorbing/radiating boundaries)

Energy Stepping, Force Stepping…

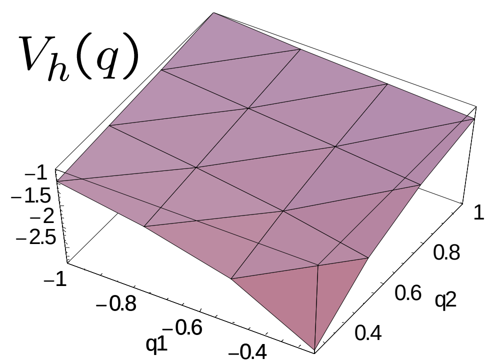
- **Main idea:** *Replace the original Lagrangian* $L(\dot{q}, q)$ *by an approximate Lagrangian* $L_h(\dot{q}, q)$ *that can be solved exactly!*
- Structural Lagrangian: $L(\dot{q}, q) = \frac{1}{2}\dot{q}^T M \dot{q} - V(q)$
- Approximate Lagrangian: $L_h(\dot{q}, q) = \frac{1}{2}\dot{q}^T M \dot{q} - V_h(q)$



Exact potential



Piecewise constant



Piecewise linear

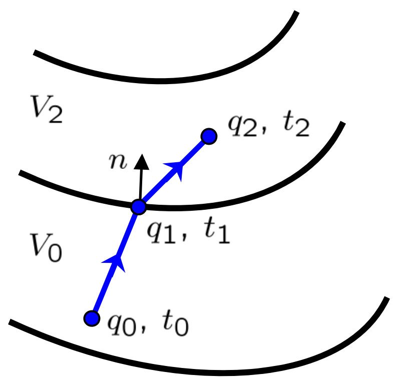
$$V_h(q) = h\lfloor h^{-1} V(q) \rfloor$$

Energy Stepping, Force Stepping…

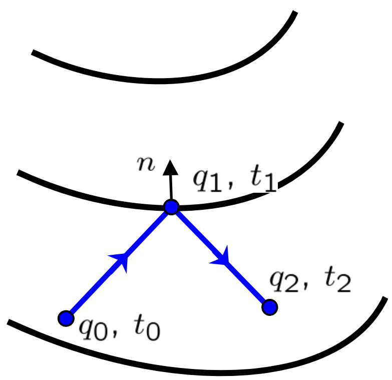
- Exact trajectories of the approximate Lagrangians:

$$V_h(q) = h\lfloor h^{-1} V(q) \rfloor$$

Piecewise constant approximation



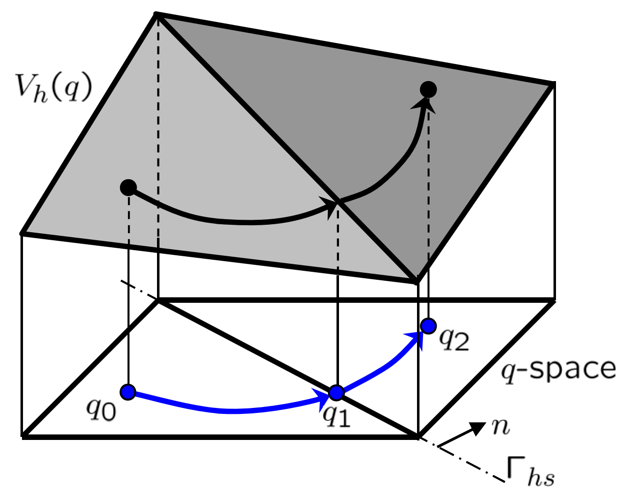
Diffraction by downhill/uphill energy step



Reflection by uphill energy step

Energy stepping

Piecewise linear approximation



System in free-fall within simplices

Force stepping

Energy Stepping – Exact trajectory

- Approximate energy:

$$V_h(q) = h\lfloor h^{-1} V(q) \rfloor$$

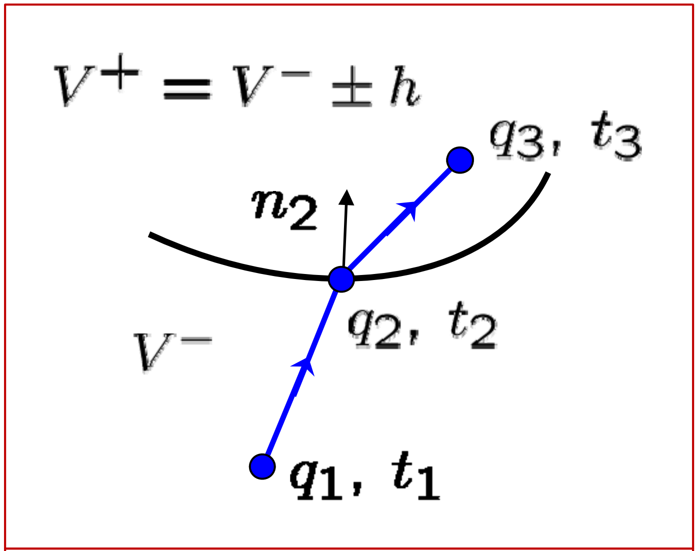
- Position update:

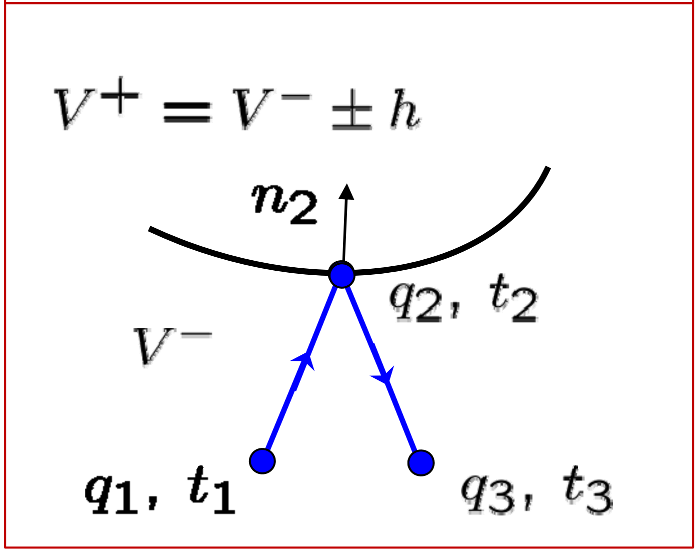
$$q_2 = q_1 + (t_2 - t_1)\dot{q}_1^+ \in h\mathbb{Z}$$

- Velocity update:

$$\dot{q}_2^+ = \dot{q}_1^+ + \lambda_2 M^{-1} n_2$$

$$\frac{1}{2}\dot{q}^{+T} M \dot{q}^+ = \frac{1}{2}\dot{q}^{-T} M \dot{q}^- + \Delta V$$





Energy Stepping – Conservation props.

- Discrete symplecticity, $\varphi_{\Delta t *}\Omega = \Omega$, verified by direct computation

Theorem. *The energy-stepping trajectories conserve all invariants of* $L(q, \dot{q}) = \frac{1}{2}\dot{q}^T M \dot{q} - V(q)$.

Proof. Consider a symmetry $\Phi : G \times Q \to Q$ such that $V \circ \Phi_g = V$, $\forall g \in G$. Note that momentum map

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

is the same for V and V_h. Note further:

$V_h \circ \Phi_g = (h\lfloor h^{-1} V \rfloor) \circ \Phi_g = h \lfloor h^{-1} V \circ \Phi_g \rfloor = h \lfloor h^{-1} V \rfloor = V_h \Rightarrow J_h = J =$ constant by Noether's theorem

Energy Stepping – Convergence

- Example of non-convergence:

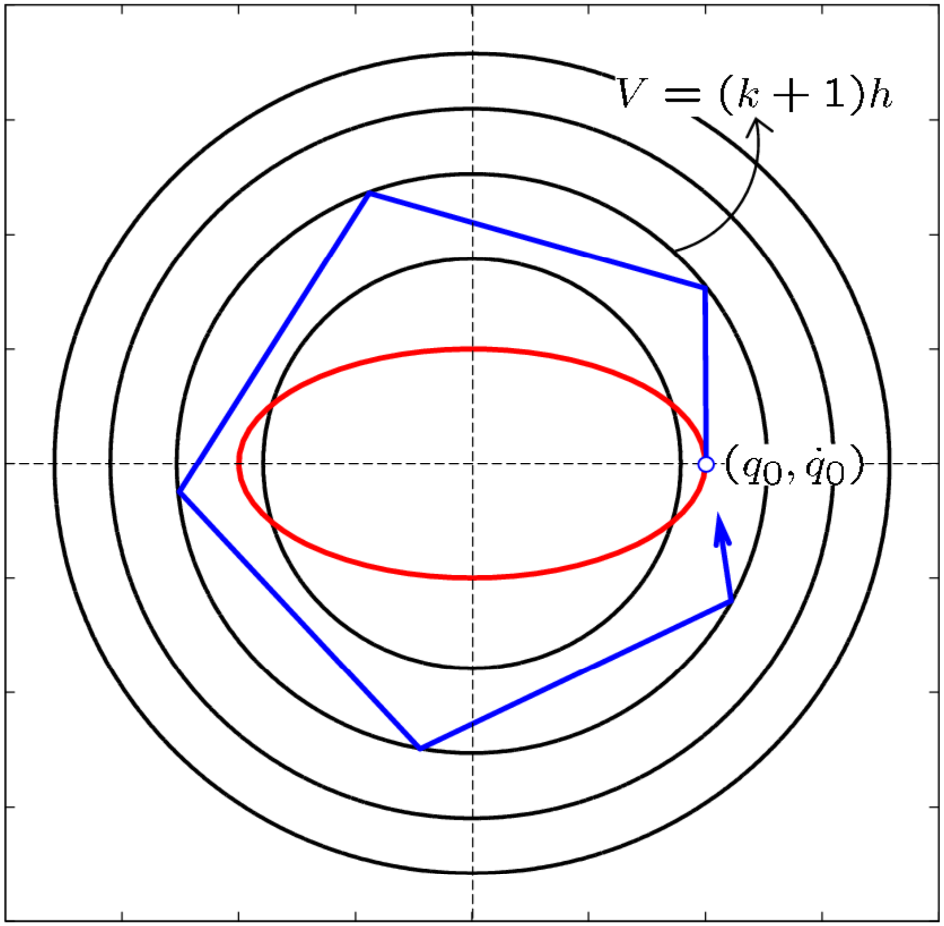
$$V = \frac{1}{2}(x^2 + y^2)$$

$$m = 1$$

$$q_0 = (1, 0)$$

$$\dot{q}_0 = (0, \gamma)$$

$$q(t) = (\cos(t), \gamma \sin(t))$$



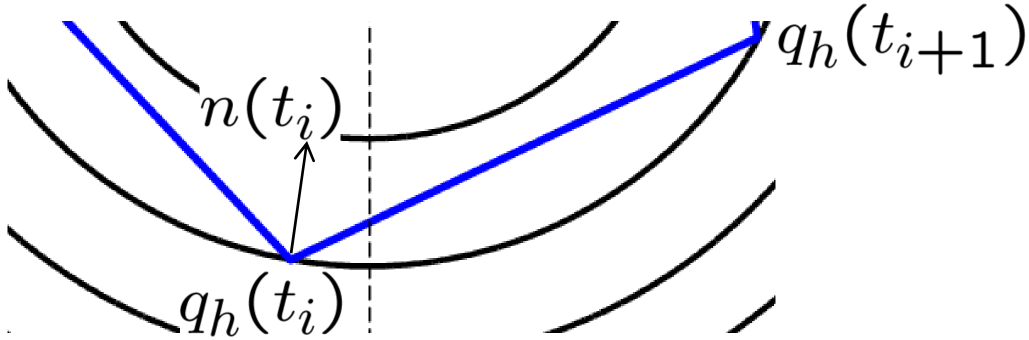
Energy Stepping – Convergence

Definition (transversality). *Let* q_h *be a sequence of energy-stepping trajectories. Let* $S(q_h) = \{t_1, \ldots, t_{N_h}\}$ *be the jump set of* $\dot{q}_h(t)$. *Then,* q_h *is transversal if*

$$\lim_{h\to 0} \min_i \frac{|n(t_i)\cdot \dot{q}_h(t_i^-)|}{\sqrt{h}} = \infty$$

and

$$\lim_{h\to 0} \max_i \frac{|q_h(t_{i+1}) - q_h(t_i)|}{\sqrt{h}} = 0.$$



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Energy Stepping – Convergence

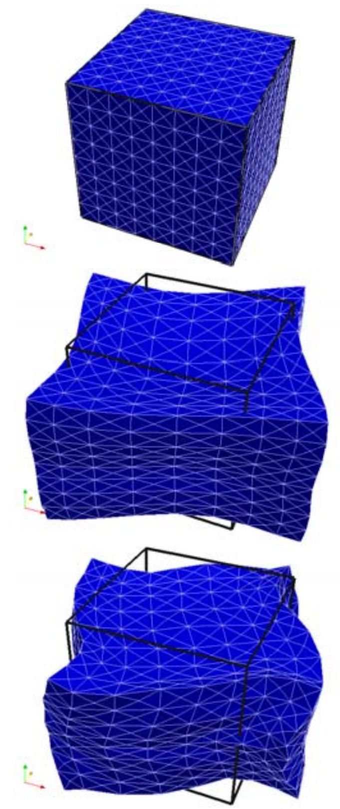
Theorem (Global convergence). *Let* q_0 *and* $\dot{q}_0$ *be given such that* $\nabla V(q_0) \cdot \dot{q}_0 \neq 0$ *and let* q_h *be the energy-stepping trajectory such that* $q_h(0) = q_0$ *and* $\dot{q}_h(0^+) = \dot{q}_0$. *Then, if the sequence* q_h *is transversal,* $q_h \to q$ *in* $W^{1,p}(0,T)$ *for each fixed* $T > 0$ *and all* $p < \infty$*, where* q *is the unique solution of the equations of motion.*

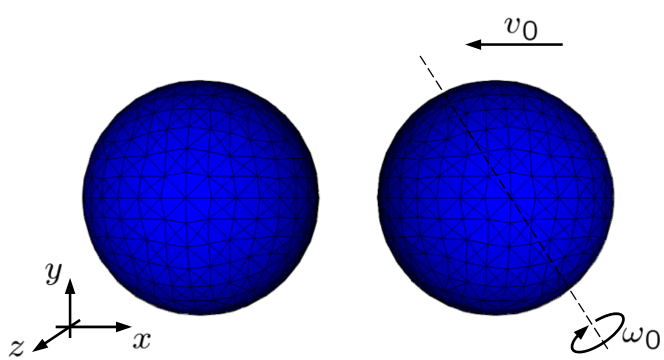
Energy stepping – Appraisal

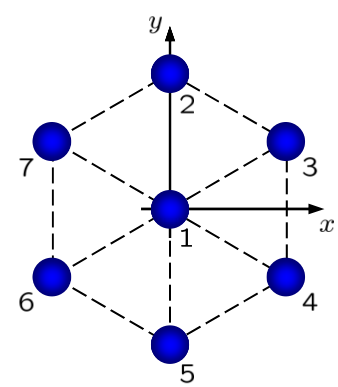
- Energy-stepping scheme is symplectic, energy-momentum time-reversible integrator with automatic selection of the time step size
- Energy-stepping automatically conserves all the invariants of the system, whether explicitly known or not (hidden symmetries)
- The exact invariants of the system, as opposed to discrete approximations thereof, are exactly conserved by energy stepping
- Convergence subject to transversality condition

Energy stepping – Examples

- Dynamics of a frozen argon cluster
- Spinning neo-Hookean cube
- Dynamic contact of deformable bodies

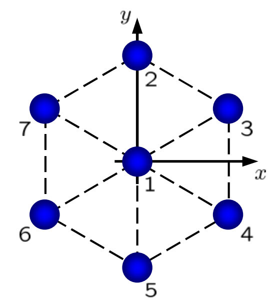


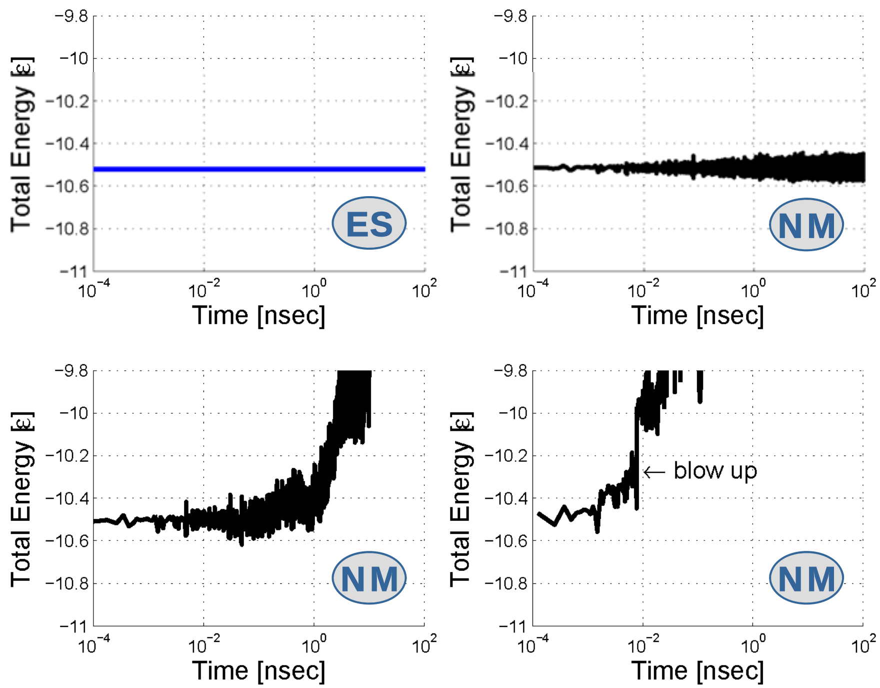




Energy stepping – Argon cluster

$$L(q,\dot q) = \underbrace{\frac{1}{2}\sum_{i=1}^{N} m_i \|\dot q_i\|^2}_{\textit{Kinetic energy}} - \underbrace{\sum_{i=1}^{N-1}\sum_{j=i+1}^{N} V\left(\left\|q_i - q_j\right\|\right)}_{\textit{Potential energy}}$$





Lennard-Jones pair potential

$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

Explicit Newmark (velocity Verlet)

$$q_{(n+1)} = q_{(n)} + \Delta t\ \dot q_{(n)} - \frac{\Delta t^2}{2} M^{-1}\nabla V(q_{(n)})$$

$$\dot q_{(n+1)} = \dot q_{(n)} - \frac{\Delta t}{2} M^{-1}\left[\nabla V(q_{(n)}) + \nabla V(q_{(n+1)})\right]$$

Total time simulated 100nsec

$$\bar{\Delta} t = 57\text{fsec},\ 87\text{fsec},\ 125\text{fsec},\ (10\text{fsec})$$

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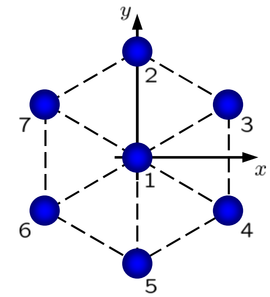
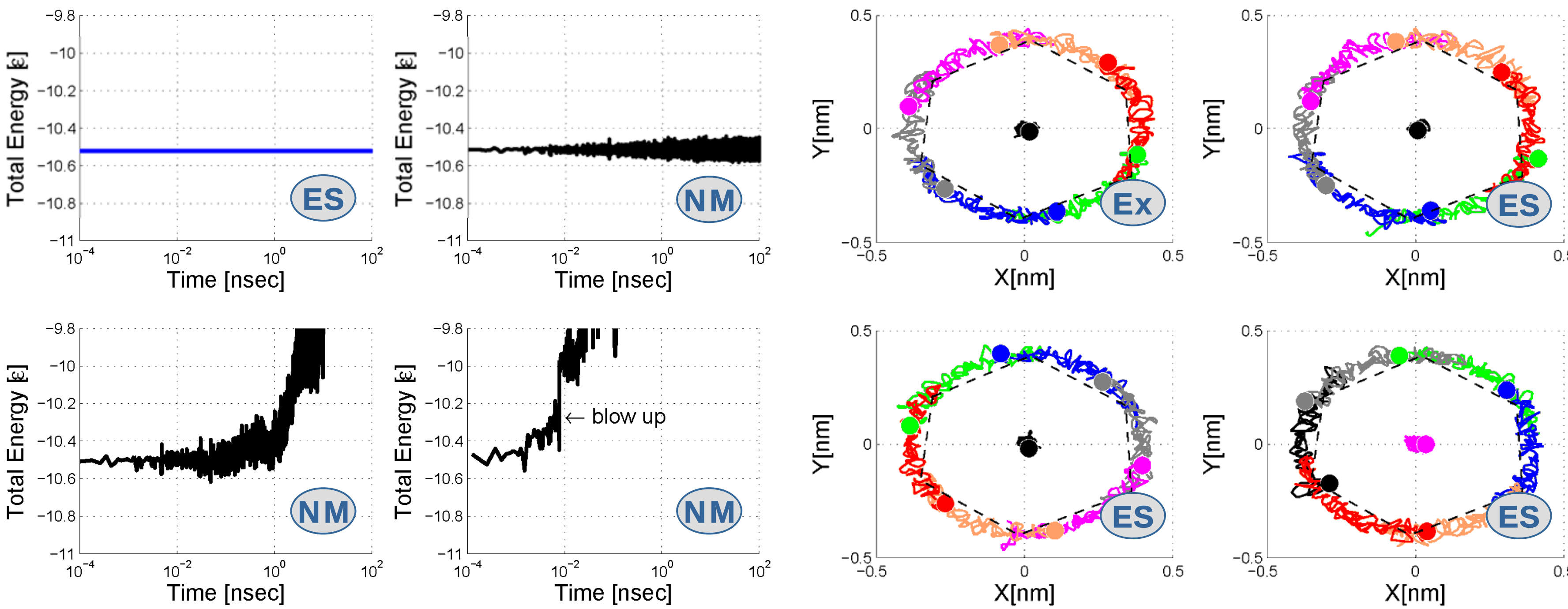
Energy stepping – Argon cluster

$$L\left(q,\dot{q}\right) = \frac{1}{2}\sum_{i=1}^{N} m_i \left\|\dot{q}_i\right\|^2 - \sum_{i=1}^{N-1}\sum_{j=i+1}^{N} V\left(\left\|q_i - q_j\right\|\right)$$





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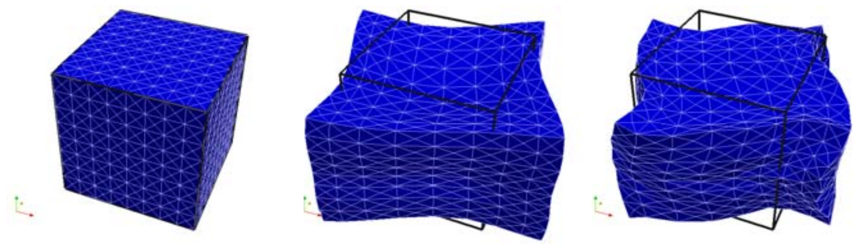
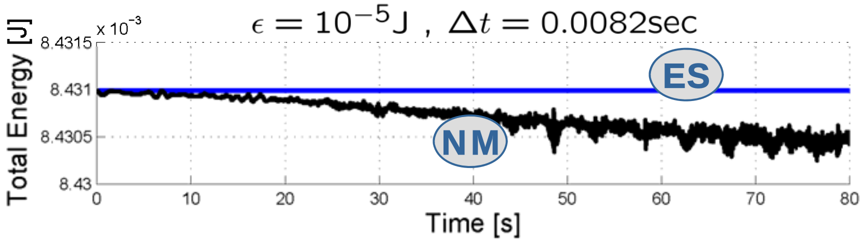
Energy stepping – Spinning cube

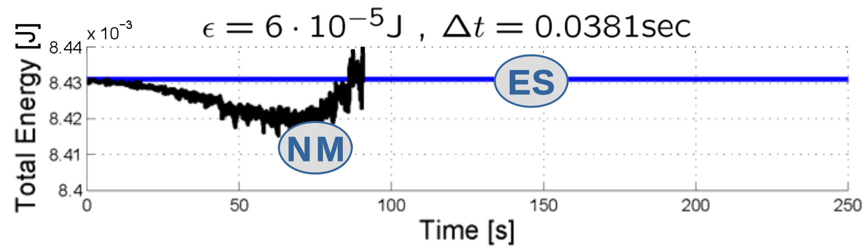
Finite element mesh: 12288 4-node tetrahedral isoparametric elements and 2969 nodes.-

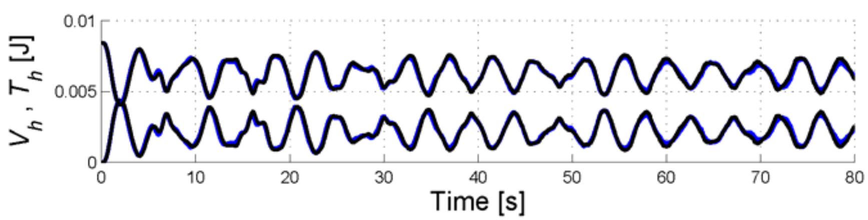
Strain-energy density:

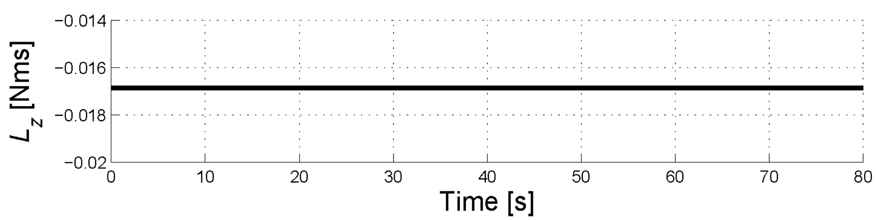
$$W(\mathbf{F}, X) = \frac{\lambda_0}{2}(\log J)^2 - \mu_0 \log J + \frac{\mu_0}{2}\,\mathrm{tr}\left(\mathbf{F}^T\mathbf{F}\right)$$

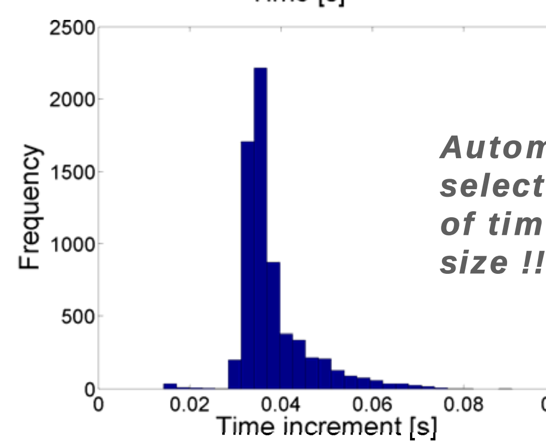












Automatic selection of time step size !!

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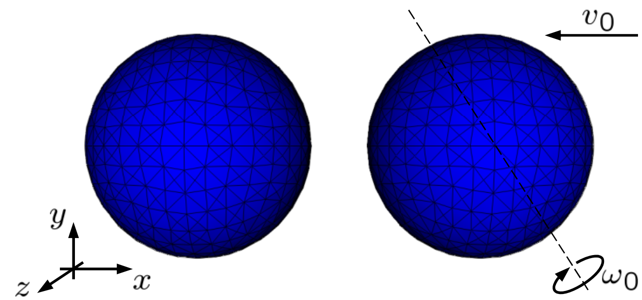
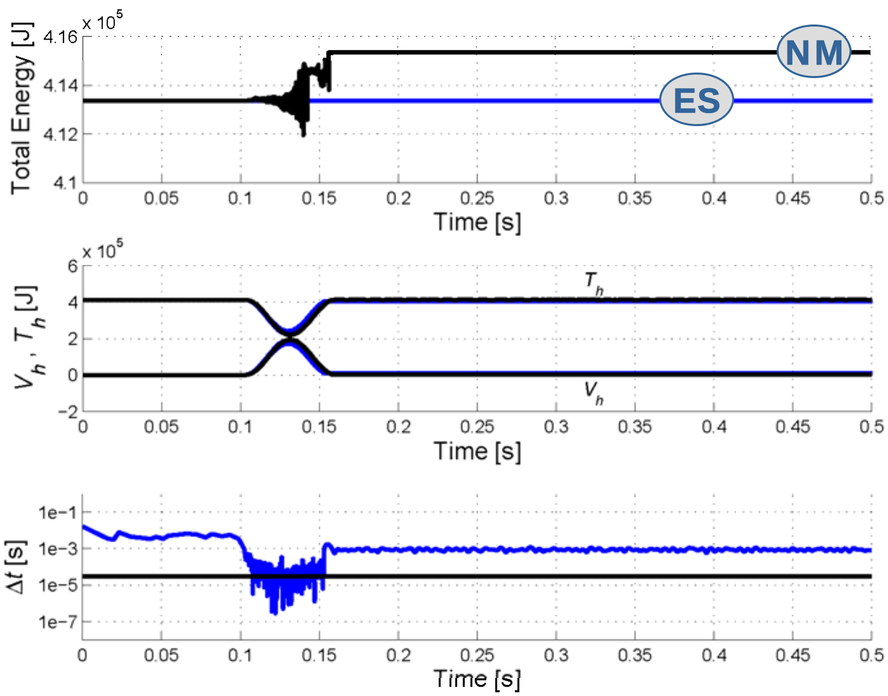
Energy stepping – Spinning cube

The ball on the left is initially in rest.

The ball on the right is set into motion with initial linear and angular velocities.





Energy-stepping $h = 10^3$J , $\bar{\Delta} t = 275\mu$sec

Explicit Newmark $\Delta t = 30\mu$sec

Complex dynamics of non-smooth contact
Hyperelastic material properties
Explicit treatment of vibrational energy

Contact duration	Coefficient of restitution
$\tau = 47.6$msec	$e = 0.964$
$\tau = 69.0$msec	$e = 1.000$

Static Hertz law // Perfectly smooth rigid bodies

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Concluding remarks

- Main idea: *Replace the original Lagrangian by an approximate one that can be solved exactly*
- Energy stepping scheme: Replace potential energy by *terraced* approximation
- Energy stepping trajectories consist of piecewise rectilinear motion, automatic time-step selection
- Energy stepping is symplectic, energy-momentum conserving, time-reversible
- Convergence subject to transversality
- Transversality does not appear to be a concern in practice for large problems, general conditions