Variational Integrators for Mechanical Systems

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Geometric Methods in Dynamics

Sponsors

- Klaus-Körper-Stiftung der Gesellschaft für Angewandte Mathematik und Mechanik (GAMM e.V.)
- Ingenieurgesellschaft Auto und Verkehr (IAV GmbH)
- Institut für Mechatronik (IfM e.V.)

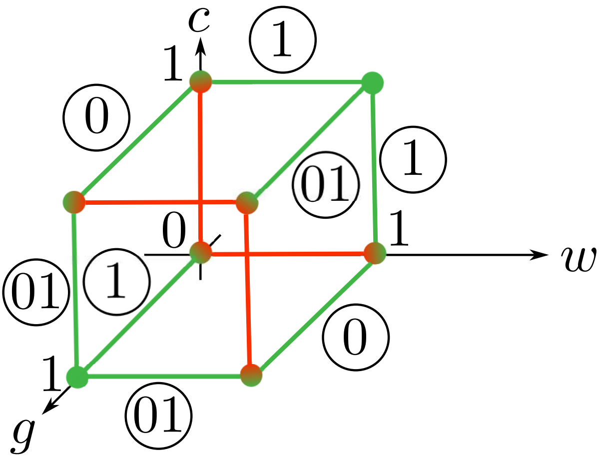
automotive engineering iav

Institut für Mechatronik

Motivation [Stewart 2009]

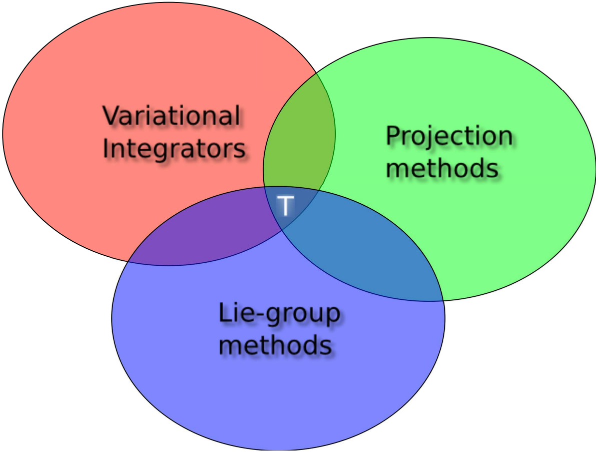
Crossing a river with a goat, a cabbage and a wolf..

Motivation [Stewart 2009]



geometric representation of its 2 solutions (7 moves each)

Geometric Time-Integration



Outline

(Non-exhaustive) Review of Variational Methods

- 1909 Ritz: *Über eine neue Methode zur Lösung gewisser Variationsprobleme der mathematischen Physik*
- 1970 Cadzow: *Discrete Calculus of Variations*
- 2000 Marsden: *Discrete Mechanics and* ***Variational Integrators***
- 2016 Desbrun, Lew, Murphey, Leyendecker, Ober-Blöbaum

Not exactly in the field of VIs but closely related are Simo & Gonzalez, Wanner & Hairer & Lubich, Reich, Betsch, Owren, Celledoni.

Technical Terms

scalar function	$\mathbb{R} \rightarrow \mathbb{R}$	$y(x) = x^2$
scalar field	$\mathbb{R}^n \rightarrow \mathbb{R}$	$y(\mathbf{x}) = x_1^2 + x_2^2$
functional	$\mathbb{D} \rightarrow \mathbb{R}$	$S[\mathbf{x}(t)] = \int_{t_a}^{t_b} \sqrt{x_1'(t)^2 + x_2'(t)^2}\,\mathrm{d}t$
vector field	$\mathbb{R}^n \rightarrow \mathbb{R}^m$	$\mathbf{y}(\mathbf{x}) = \begin{bmatrix} x_1^2 + x_2^2 \\ x_1^2 - x_2^2 \end{bmatrix}$
operator	$\mathbb{D} \rightarrow \mathbb{D}$	$D[y(x)] = \frac{\mathrm{d}y}{\mathrm{d}x}$

Directional Derivatives

recalling analysis for scalar functions and scalar fields

$y(x)$	$\frac{\mathrm{d}y}{\mathrm{d}x} = \lim_{\varepsilon\to 0} \frac{y(x+\varepsilon)-y(x)}{\varepsilon}$
$y(x) = x^2$	$\frac{\mathrm{d}y}{\mathrm{d}x} = 2x$
	$x_0 = 2 \rightsquigarrow \left.\frac{\mathrm{d}y}{\mathrm{d}x}\right\|_{x_0} = 4$
$y(\mathbf{x})$	$\frac{\mathrm{d}y}{\mathrm{d}\mathbf{n}} = \lim_{\varepsilon\to 0} \frac{y(\mathbf{x}+\varepsilon\mathbf{n})-y(\mathbf{x})}{\varepsilon}$
$y(\mathbf{x}) = x_1^2 + x_2^2$	$\frac{\mathrm{d}y}{\mathrm{d}\mathbf{n}} = \begin{bmatrix} 2x_1 \\ 2x_2 \end{bmatrix} \cdot \begin{bmatrix} n_1 \\ n_2 \end{bmatrix}$
	$\mathbf{x}_0 = \begin{bmatrix} 1 \\ 1 \end{bmatrix},\ \mathbf{n}_0 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \rightsquigarrow \left.\frac{\mathrm{d}y}{\mathrm{d}\mathbf{n}}\right\|_{\mathbf{x}_0,\mathbf{n}_0} = 2$

Directional Derivatives

variations are directional derivatives of functionals

$$J[y(x)]$$

$$\delta J[y,\eta] = \lim_{\varepsilon\to 0} \frac{J[y(x)+\varepsilon\eta(x)]-J[y(x)]}{\varepsilon}$$

$$J[y(x)] = \int_0^{\frac{\pi}{2}} y(x)^2 \,\mathrm{d}x$$

$$\delta J[y,\eta] = \int_0^{\frac{\pi}{2}} 2y(x)\eta(x)\,\mathrm{d}x$$

$$y_0(x) = \sin(x),\ \eta_0(x) = \cos(x)$$

$$\rightsquigarrow \delta J[y_0,\eta_0] = 1$$

Extrema of Functionals

First order *necessary* conditions for functionals of type

$$J[y(t),t] = \int_a^b L\Big(t, y(t), y'(t)\Big)\,\mathrm{d}t$$

and admissible perturbations $\eta(a) = \eta(b) = 0$

$$\begin{aligned}
\delta J[y,\eta] &= \int_a^b L_y\eta + L_{y'}\eta'\,\mathrm{d}t = 0 \\
&= \int_a^b L_y\eta - \left(\frac{\mathrm{d}}{\mathrm{d}t}L_{y'}\right)\eta\,\mathrm{d}t + \left|L_{y'}\eta\right|_a^b = 0 \\
&= \int_a^b \left(L_y\eta - \frac{\mathrm{d}}{\mathrm{d}t}L_{y'}\right)\eta\,\mathrm{d}t = 0
\end{aligned}$$

are the Euler-Lagrange-equations $L_y = \frac{\mathrm{d}}{\mathrm{d}t}L_{y'}$.

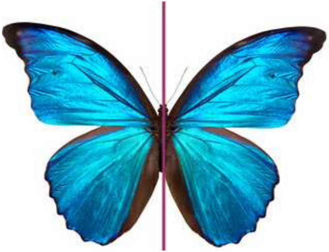
Extrema of Functionals

Remarks

- There are a lot of applications in physics and engineering. The classical problems are Dido's problem, Brachystochrone, Catenary, Geodetics, Minimal surfaces, ...
- The evaluation of *sufficient* conditions (of Legendre and Jacobi) for extrema of functionals is more involved than those of functions and skipped here.

Power of Symmetries [Mahajan 2014]

http://wild.maths.org



Symmetries are not only beautiful, but also provide practical tools.

example solve the heat equation (selectively) without calculations

Noether's Theorem [Levi 2014]

If the Lagrangian is invariant under action of a one-parameter family of diffeomorphism h^s (e.g. $h^s\mathbf{q} = \mathbf{q} + s\mathbf{e}$)

$$L\left(h^s\mathbf{q}(t), \frac{\mathrm{d}}{\mathrm{d}t}\Big(h^s\mathbf{q}(t)\Big)\right) = L\Big(\mathbf{q}(t), \dot{\mathbf{q}}(t)\Big),$$

then

$$L_{\dot{\mathbf{q}}} \cdot \frac{\mathrm{d}}{\mathrm{d}s}\bigg|_{s=0} h^s\mathbf{q} = \text{constant}.$$

example

$L = \frac{1}{2}(\dot{x}_1^2 + \dot{x}_2^2) - \frac{1}{2}c(x_2 - x_1)^2$ and $h^s\mathbf{x} = \mathbf{x} + s[1, 1]^T$

$$\rightsquigarrow \begin{bmatrix} m_1\dot{x}_1 \\ m_2\dot{x}_2 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 1 \end{bmatrix} = p_{\text{total}} = \text{const.}$$

Noether's Theorem [Levi 2014]

sketch of proof

If the Lagrangian is not altered, neither is the action (here defined by start- and end-position rather than start-position and -momentum)

$$S(t_1, h^s\mathbf{q}_1) - S(t_0, h^s\mathbf{q}_0) = S(t_1, \mathbf{q}_1) - S(t_0, \mathbf{q}_0)$$

After derivation with respect to s

$$\underbrace{S_{\mathbf{q}_1}}_{L_{\dot{\mathbf{q}}|t_1}} \cdot \left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=0} h^s\mathbf{q}_1 - \underbrace{S_{\mathbf{q}_0}}_{L_{\dot{\mathbf{q}}|t_0}} \cdot \left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=0} h^s\mathbf{q}_0 = 0$$

Since t_1 is arbitrary the expression $L_{\dot{\mathbf{q}}} \cdot \left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=0} h^s\mathbf{q}_1$ must remain constant. Only left to show is $S_{\mathbf{q}_1} = L_{\dot{\mathbf{q}}|_{t_1}}$.

Noether's Theorem [Levi 2014]

Let the critical function be parametrized by its end position

$$\mathbf{q}(t) = \mathbf{Q}(t, t_1, \mathbf{q}_1)$$

insert into the action function

$$S(t_1, \mathbf{q}_1) = \int_{t_0}^{t_1} L(\mathbf{Q}, \dot{\mathbf{Q}})\,\mathrm{d}t$$

and differentiate by $\mathbf{q}_1$

$$\begin{aligned} S_{\mathbf{q}_1} &= \int_{t_0}^{t_1} L_{\mathbf{q}} \mathbf{Q}_{\mathbf{q}_1} + L_{\dot{\mathbf{q}}} \dot{\mathbf{Q}}_{\mathbf{q}_1}\,\mathrm{d}t \\ &= \int_{t_0}^{t_1} \left(L_{\mathbf{q}} - \frac{\mathrm{d}}{\mathrm{d}t} L_{\dot{\mathbf{q}}} \right) \mathbf{Q}_{\mathbf{q}_1}\,\mathrm{d}t + |L_{\dot{\mathbf{q}}} \mathbf{Q}_{\mathbf{q}_1}|_{t_0}^{t_1} \\ &= L_{\dot{\mathbf{q}}}\big|_{t=t_1}. \end{aligned}$$

Chemnitz

..an industrial city with about 250.000 inhabitants (2015).

Point of Departure

HAMILTON'S PRINCIPLE rules the classical mechanics

$$\delta \int_{t_b}^{t_e} L(\mathbf{q}, \dot{\mathbf{q}})\,\mathrm{d}t = 0 \qquad \text{with} \qquad L = T(\mathbf{q}, \dot{\mathbf{q}}) - V(\mathbf{q}),$$

typically used for equations of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{\mathbf{q}}}\right) - \frac{\partial L}{\partial \mathbf{q}} = 0,$$

which are often nonlinear and solved numerically.

The Lagrangian $L(\mathbf{q}, \dot{\mathbf{q}})$ lives on tangent bundle $L : TM \to \mathbb{R}$ of the configuration manifold M.

Point of Departure

Equivalently, the system can be brought into Hamiltonian form by the Legendre Transformation

$$H(\mathbf{q}, \mathbf{p}) = \mathbf{p} \cdot \dot{\mathbf{q}} - L.$$

Due to substitution of variables, presuming $\frac{\partial^2 L}{\partial \dot{\mathbf{q}} \partial \dot{\mathbf{q}}}$ regular

$$\mathbf{p}(\mathbf{q}, \dot{\mathbf{q}}) = \frac{\partial L}{\partial \dot{\mathbf{q}}}.$$

The Hamiltonian $H(\mathbf{q}, \mathbf{p})$ lives on co-tangent bundle $H : T^*M \rightarrow \mathbb{R}$ of the configuration manifold M.

The equations of motions then become

$$\begin{bmatrix} \dot{\mathbf{q}} \\ \dot{\mathbf{p}} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial \mathbf{q}} \\ \frac{\partial H}{\partial \mathbf{p}} \end{bmatrix}.$$

Point of Departure

For the simple pendulum

$$L = \frac{1}{2}\dot{\varphi}^2 + \cos\varphi$$

the equations of motion are either (Lagrangian form)

$$\ddot{\varphi} + \sin\varphi = 0,$$

with $\varphi(0) = \varphi_0,\ \dot{\varphi}(0) = \dot{\varphi}_0$, or (Hamiltonian form)

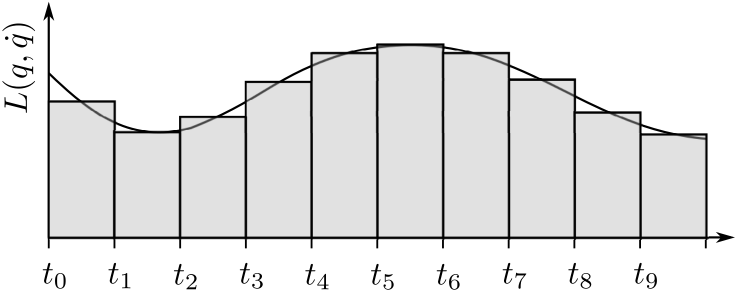
$$\begin{aligned} \dot{\varphi} &= p \\ \dot{p} &= -\sin\varphi \end{aligned}$$

with $\varphi(0) = \varphi_0 \qquad p(0) = p_0$.

Idea behind Variational Integrators

"Approximate the action instead of the equations of motion"

A.Lew



general advantages

- robustness and excellent long-time behavior
- symplecticity
- backward error analysis

VI for Conservative Systems

[Marsden 2000]

1. Approximation of the state variables in time

$$\mathbf{q}(t) \approx \mathbf{q}^d(t) = \frac{t_{k+1} - t}{h}\mathbf{q}_k + \frac{t - t_k}{h}\mathbf{q}_{k+1}.$$

2. Time-step-wise quadrature of the action-integral

$$\begin{aligned}\Delta S &= \int_{t_k}^{t_{k+1}} L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t)\,\mathrm{d}t \\ &\approx \int_{t_k}^{t_{k+1}} L(\mathbf{q}^d(t), \dot{\mathbf{q}}^d(t), t)\,\mathrm{d}t \\ &\approx hL(\mathbf{q}^d(t_{k+1/2}), \dot{\mathbf{q}}^d(t_{k+1/2}), t_{k+1/2}) = L_d.\end{aligned}$$

$L_d(\mathbf{q}_k, \mathbf{q}_{k+1})$ lives on discrete state space $L_d : M \times M \to \mathbb{R}$.

VI for Conservative Systems

[Marsden 2000]

stationarity condition of the discrete action sum

$$S \approx S_d = \sum_{k=0}^{N-1} L_d(\mathbf{q}_k, \mathbf{q}_{k+1})$$

yields discrete Euler-Lagrange equations

$$\begin{aligned} \delta S_d \quad = \quad & \cancel{D_1 L_d(\mathbf{q}_0, \mathbf{q}_1)\delta q_0} \\ & + D_2 L_d(\mathbf{q}_0, \mathbf{q}_1)\delta q_1 + D_1 L_d(\mathbf{q}_1, \mathbf{q}_2)\delta q_1 \\ & + D_2 L_d(\mathbf{q}_1, \mathbf{q}_2)\delta q_2 + D_1 L_d(\mathbf{q}_2, \mathbf{q}_3)\delta q_2 \\ & \ldots \\ & + \cancel{D_2 L_d(\mathbf{q}_{N-1}, \mathbf{q}_N)\delta q_N} = 0. \end{aligned}$$

D_i denotes derivative with respect to the i.th argument, i.e. $D_1 L_d(\mathbf{q}_k, \mathbf{q}_{k+1}) = \frac{\partial L_d}{\partial \mathbf{q}_k}$, $D_2 L_d(\mathbf{q}_k, \mathbf{q}_{k+1}) = \frac{\partial L_d}{\partial \mathbf{q}_{k+1}}$.

VI for Conservative Systems

[Marsden 2000]

The DEL determine $\mathbf{q}_k,\ \mathbf{q}_{k-1} \rightsquigarrow \mathbf{q}_{k+1}$ implicitly by

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

On one hand the I.C. $\mathbf{q}_0$, $\dot{\mathbf{q}}_0$ correspond to the momenta

$$\mathbf{p}_0 = \left.\frac{\partial L}{\partial \dot{\mathbf{q}}}\right|_{\mathbf{q}_0, \dot{\mathbf{q}}_0}$$

on the other hand the velocity approximation corresponds to

$$\mathbf{p}_{1/2} = \left.\frac{\partial L}{\partial \dot{\mathbf{q}}}\right|_{\mathbf{q}_{1/2}, \dot{\mathbf{q}}_{1/2}}$$

correction by the acting forces between $t_0 \dots t_0 + h/2$

$$\mathbf{p}_0 = \underline{D_2 L(\mathbf{q}_0, \dot{\mathbf{q}}) = -D_1 L_d(\mathbf{q}_0, \mathbf{q}_1)} = \mathbf{p}_{1/2} - \frac{h}{2} \left.\frac{\partial L}{\partial \mathbf{q}}\right|_{\mathbf{q}_{1/2}}$$

to be detailed later (discrete Legendre Transform).

Example

1DoF system (dimensionless), e.g. simple pendulum

$$L = \frac{1}{2}\dot{q}^2 - V(q)$$

with linear approximations for the time step $t = 0 \dots h$

$$q \approx q^d = \frac{h-t}{h} q_0 + \frac{t}{h} q_1 \qquad \text{and} \qquad \dot{q} \approx \dot{q}^d = \frac{q_1 - q_0}{h}$$

and trapezoidal rule for quadrature

$$\int_0^h L(q^d, \dot{q}^d) \approx \frac{h}{2} L(q_0, \dot{q}^d) + \frac{h}{2} L(q_1, \dot{q}^d) = L_d$$

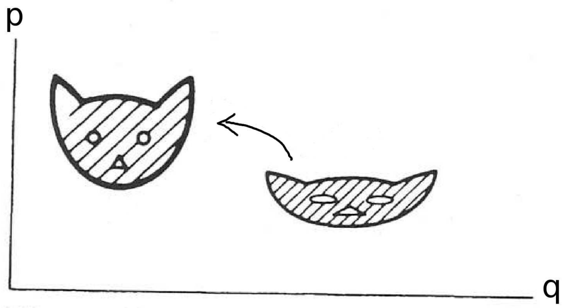
results in the popular Störmer-Verlet scheme [Verlet1967].

$$\delta S_d = 0 \quad \leadsto \quad \begin{cases} p_0 = \dot{q}^d + \frac{h}{2}\frac{\partial V}{\partial q}(q_0) & \leadsto q_1 \\ p_1 = \dot{q}^d - \frac{h}{2}\frac{\partial V}{\partial q}(q_1) & \leadsto p_1 \end{cases}$$

Symplecticity

[Arnold 1974]

The obligatory picture is (Vladimir Igorevich) Arnold's cat

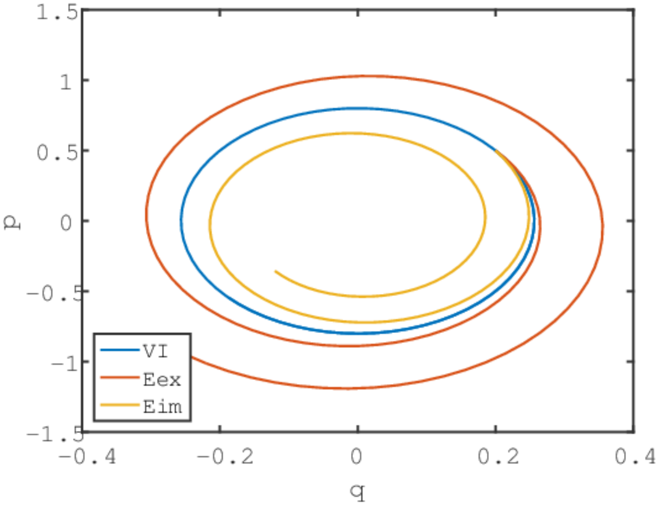


Sets of initial conditions preserve their volumes in phase space while flowing according to the equations of motion.

Confer with mapping reference configuration → current configuration in static continuum mechanics.

Symplecticity

Advantages for numerical simulations



Simulations of a simple pendulum by various methods

Discrete Legendre Transform

[Lew 2004]

Similarly to the continous case, there is a discrete momentum definition.

$$\begin{aligned} \mathbf{p}_k &= -D_1 L_d(\mathbf{q}_k, \mathbf{q}_{k+1}) \\ \mathbf{p}_{k+1} &= D_2 L_d(\mathbf{q}_k, \mathbf{q}_{k+1}) \end{aligned}$$

whose continuity is enforced by the DEL.

Hint, express derived quantities, such as velocities or energies, as functions of $\mathbf{q}_k$ and $\mathbf{p}_k$, instead of evaluating the approximations $\mathbf{q}^d(t)$!

Discrete Noether Theorem

If there is a one-parameter group h^s that leaves

$$L_d(h^s\mathbf{q}_k, h^s\mathbf{q}_{k+1}) = L_d(\mathbf{q}_k, \mathbf{q}_{k+1})$$

invariant, then there is an invariant of the dynamics

$$I(\mathbf{q}_k, \mathbf{p}_k) = \mathbf{p}_k \cdot \frac{\mathrm{d}}{\mathrm{d}s} h^s\mathbf{q}_k = \text{constant.}$$

example: two masses connected by a spring

$$L = \tfrac{1}{2}m(\dot{x}^2 + \dot{y}^2) - \tfrac{1}{2}c(y-x)^2, \qquad h^s\mathbf{q} = \mathbf{q} + [s, s]^T$$

$$\mathbf{p_0} = -D_1L_d = \begin{bmatrix} m\frac{x_1-x_0}{h} - \frac{h}{2}c(y_{1/2} - x_{1/2}) \\ m\frac{y_1-y_0}{h} + \frac{h}{2}c(y_{1/2} - x_{1/2}) \end{bmatrix}$$

$$\mathbf{p_1} = D_2L_d = \begin{bmatrix} m\frac{x_1-x_0}{h} + \frac{h}{2}c(y_{1/2} - x_{1/2}) \\ m\frac{y_1-y_0}{h} - \frac{h}{2}c(y_{1/2} - x_{1/2}) \end{bmatrix}$$

$$I = m\frac{x_1 - x_0}{h} + m\frac{y_1 - y_0}{h}$$

Forcing and Dissipation

[Marsden 2000]

Discrete Lagrange-D'Alembert principle, derived from time-continous formulation

$$\delta \int_{t_b}^{t_e} L \, \mathrm{d}t + \int_{t_b}^{t_e} \delta W^{\mathrm{nc}} \, \mathrm{d}t = \sum_{k=0}^{N-1} \delta \int_{t_k}^{t_{k+1}} L \, \mathrm{d}t + + \int_{t_k}^{t_{k+1}} \delta W^{\mathrm{nc}} \, \mathrm{d}t = 0$$

L as before and virtual work of non-conservative forces by

$$\int_{t_k}^{t_{k+1}} \delta W^{\mathrm{nc}} \, \mathrm{d}t = \int_{t_k}^{t_{k+1}} \mathbf{F}(t) \cdot \delta \mathbf{q}(t) \, \mathrm{d}t \approx \int_{t_k}^{t_{k+1}} \mathbf{F}(t) \cdot \delta \mathbf{q}^d(t) \, \mathrm{d}t$$

$$\approx h \mathbf{F}(t_{k+1/2}) \cdot \delta \mathbf{q}^d(t_{k+1/2}) = \mathbf{F}_k^- \delta \mathbf{q}_k + \mathbf{F}_{k+1}^+ \delta \mathbf{q}_{k+1}.$$

DEL arranged in *position-momentum* form

$$\begin{aligned} \mathbf{p}_k &= -D_1 L_d(\mathbf{q}_k, \mathbf{q}_{k+1}) - \mathbf{F}_k^-(\mathbf{q}_k, \mathbf{q}_{k+1}) \\ \mathbf{p}_{k+1} &= D_2 L_d(\mathbf{q}_k, \mathbf{q}_{k+1}) + \mathbf{F}_k^+(\mathbf{q}_k, \mathbf{q}_{k+1}). \end{aligned}$$

Alternative Approach

[Vujanovic 1988]

For linear systems with damping

$$\begin{aligned} \ddot{x} + 2D\dot{x} + \omega_0^2 x &= 0 \\ L &= \frac{1}{2}(\dot{x}^2 - \omega_0^2 x^2)\, e^{2Dt}, \end{aligned}$$

or forcing

$$\begin{aligned} \ddot{x} + \omega_0^2 x &= a \cos \Omega t \\ L &= \frac{1}{2}\left(\dot{x} + \frac{a\Omega \sin \Omega t}{\omega_0^2 - \Omega^2}\right)^2 - \frac{\omega_0^2}{2}\left(x - \frac{a \cos \Omega t}{\omega_0^2 - \Omega^2}\right)^2 . \end{aligned}$$

Generally seems the inverse problem of the calculus of variations to be an interesting approach.

Geometry of Constraints

Extrema are at points where the gradient of the cost function is normal to the constraint surface

$$\nabla f(\mathbf{x}_0) = -\lambda \nabla \phi(\mathbf{x}_0).$$

Reactions forces are different from external forces, as the constraints have to be fulfilled exactly and not only in some integral sense!

VI for Constrained Systems

[Marsden 2000]

Basically it works to enforce the constraints on position level only, better is enforcement on position *and* momentum level.

Iteration equations enforce constraint $\phi = 0$

$$\begin{aligned} \mathbf{0} &= \mathbf{p}_k + D_1 L_d(\mathbf{q}_k, \mathbf{q}_{k+1}) - \lambda_k \nabla\phi(\mathbf{q}_k) \\ 0 &= \phi(\mathbf{q}_{k+1}), \end{aligned}$$

while update-equations enforce “hidden” constraint ($\dot{\phi} = 0$)

$$\begin{aligned} \mathbf{p}_{k+1} &= D_2 L_d(\mathbf{q}_k, \mathbf{q}_{k+1}) - \tilde{\lambda}_{k+1} \nabla\phi(\mathbf{q}_{k+1}) \\ 0 &= \nabla\phi(\mathbf{q}_{k+1}) \cdot \frac{\partial H}{\partial \mathbf{p}}(\mathbf{q}_{k+1}, \mathbf{p}_{k+1}). \end{aligned}$$

Alternatively, eliminate the Lagrange-multipliers by the nullspace method [Betsch2005], for VI [Leyendecker2008].

Example

[Bruels 2011]

Heavy top

Euler-Parameters

Parametrization by Euler-parameters (unit quaternions)

- ✓ free of singularities
- ϟ additional constraint $q_0^2 + q_1^2 + q_2^2 + q_3^2 = 1$
- ϟ mysterious momenta $p_i = \dfrac{\partial L}{\partial \dot{q}_i} = ?$

Example

[Betsch 2006]

Crucial point ist the kinetic energy

$$T = \frac{1}{2}\dot{\mathbf{q}} \cdot \mathbf{M}_4 \dot{\mathbf{q}},$$

with the rank-one augmented mass matrix

$$\mathbf{M}_4 = 4\mathbf{G}(\mathbf{q})^T \mathbf{J}\mathbf{G}(\mathbf{q}) + 2\mathrm{tr}(\mathbf{J})\mathbf{q} \otimes \mathbf{q},$$

where $\mathbf{G}(\mathbf{q})$ relates to the convective angular velocity

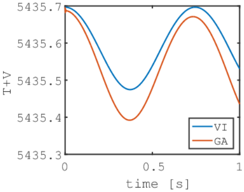
$$\boldsymbol{\Omega} = 2\mathbf{G}(\mathbf{q})\dot{\mathbf{q}} \qquad \dot{\mathbf{q}} = \frac{1}{2}\mathbf{G}(\mathbf{q})^T \boldsymbol{\Omega}.$$

Potential energy as usual

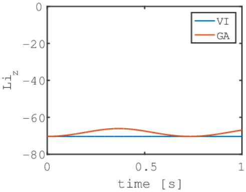
$$V = mg\mathbf{e}_z \cdot \mathbf{x}_s = mg\mathbf{e}_z \cdot \mathbf{R}(\mathbf{q})\mathbf{X}_s.$$

Example

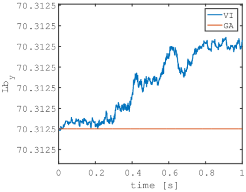
The VI is compared with the generalized-α method $(h = 10^{-}3\text{s},\ \rho = 0.9)$ for the fast spinning heavy top.



total mech. energy



ang. mom. L_z



ang. mom. L_3

TU Chemnitz

www.panoramio.com

.. a technical university with about 11.000 students (2015).

Discrete Lagrangian

[Marsden 2000]

1. approximation of the state variables in time

$$\mathbf{q}(t) \approx \mathbf{q}^d(t) = \sum_{n=0}^{p} M_n(t)\mathbf{q}_{k+n/p}$$

2. time-step-wise quadrature of the action-integral..

$$\begin{aligned} \Delta S &= \int_{t_k}^{t_{k+1}} L\Big(\mathbf{q}(t), \dot{\mathbf{q}}(t), t\Big)\,\mathrm{d}t \\ &\approx \int_{t_k}^{t_{k+1}} L\Big(\mathbf{q}^d(t), \dot{\mathbf{q}}^d(t), t\Big)\,\mathrm{d}t \\ &\approx \sum_{m=1}^{g} w_m L\Big(\mathbf{q}^d(t_m), \dot{\mathbf{q}}^d(t_m), t_m\Big) = L_d \end{aligned}$$

Forced Discrete Lagrange-D'Alembert-Principle

[Marsden 2000]

..and the virtual work of the nonconservative forces

$$\delta W^{\mathrm{nc}} = \int_{t_k}^{t_{k+1}} \mathbf{F} \cdot \delta \mathbf{q} \, \mathrm{d}t \approx \int_{t_k}^{t_{k+1}} \mathbf{F} \cdot \delta \mathbf{q}^d \, \mathrm{d}t$$

$$\approx \sum_{m=1}^{g} w_m \mathbf{F}(t_m) \cdot \delta \mathbf{q}^d(t_m) = \sum_{n=0}^{p} \mathbf{F}^d_{k+n/p} \delta \mathbf{q}^d_{k+n/p}$$

yield DEL (position-momentum form)

$$\mathbf{p}_k = -D_1 L_d(\mathbf{q}_k, \mathbf{q}_{k+1/p} \dots, \mathbf{q}_{k+1}) - \mathbf{F}^d_k$$

$$\mathbf{0} = D_2 L_d(\mathbf{q}_k, \mathbf{q}_{k+1/p} \dots, \mathbf{q}_{k+1}) + \mathbf{F}^d_{k+1/p}$$

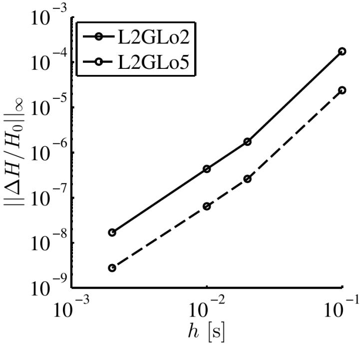
$$\dots$$

$$\mathbf{0} = D_p L_d(\mathbf{q}_k, \mathbf{q}_{k+1/p} \dots, \mathbf{q}_{k+1}) + \mathbf{F}^d_{k+\frac{p-1}{p}}$$

$$\mathbf{p}_{k+1} = D_{p+1} L_d(\mathbf{q}_k, \mathbf{q}_{k+1/p} \dots, \mathbf{q}_{k+1}) + \mathbf{F}^d_{k+1}$$

Order Analysis

[Ober-Blöbaum & Saake 2013]



Quadratic polynomial approximation numerically integrated by different order

Approximation by polynomial of degree p and a quadrature based on $p+1$ points enables the maximal possible order $2p$.

Backward Error Analysis

[Hairer & Wanner & Lubich 2006]

Rather than considering how closely the approximated trajectories match the exact ones, it is now considered how closely the discrete Lagrangian (Hamiltonian) matches the ideal one.

Backward error analysis reveals discrete time paths as exact solutions of a nearby Hamiltonian

$$\tilde{H}(q,p) = H(q,p) + hg_1(q,p) + h^2 g_2(q,p) + \dots$$

Notion of Thermacy

[Helmholtz 1884]

The concept of *thermacy*, also known as thermal displacements, gives heat transfer the same mathematical structure as mechanical motion.

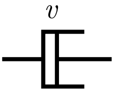
	mechanical	thermal
gen. coord.	x	α
gen. vel.	$v = \dot{x}$	$\vartheta = \dot{\alpha}$
Lagrangian	$L = \frac{1}{2} m \dot{x}^2$	$L = \frac{1}{2} \frac{k}{\vartheta_r} (\dot{\alpha} - \vartheta_r)^2$
gen. momentum	$p = \frac{\partial L}{\partial \dot{x}}$	$s = \frac{\partial L}{\partial \dot{\alpha}}$
eq. of motion	$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial x} = 0$	$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{\alpha}}\right) - \frac{\partial L}{\partial \alpha} = 0$

Discrete Model Components

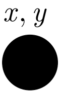
[Romero 2009]

generalized positions $\mathbf{q}$	**generalized momenta $\mathbf{p}$**	**further dependencies**
position $x,\ y$	momentum $p_x,\ p_y$	length $l(x, y)$
thermacy α	entropy s	temperature $\vartheta = \dot{\alpha}$
int. variable v	$\frac{\partial \psi}{\partial v} = 0$	non-equilibrium force $\dot{p}_v$

elastic stiffness K
thermoelastic coupling β
heat capacity k



viscosity η
relaxation time $\tau = \frac{\eta}{2\mu}$



mass m

Variational Principle for Thermo-Viscoelasticity

[Maugin 2006]

$$\delta \sum_{k=0}^{N-1} \left(\int_{t_k}^{t_{k+1}} (T - \psi)\, \mathrm{d}t \right) + \sum_{k=0}^{N-1} \left(\int_{t_k}^{t_{k+1}} \delta W^{\mathrm{nc}}\, \mathrm{d}t = 0 \right)$$

mass	kinetic energy	$T = \frac{1}{2} m(\dot{x}^2 + \dot{y}^2)$
spring	elastic strain energy	$\psi_e = \dfrac{K}{2 l_0^2}(l - l_0)^2$
	thermoelastic coupling	$\psi_{te} = -\beta(\vartheta - \vartheta_r)\dfrac{l - l_0}{l_0}$
	heat capacity	$\psi_t = -\dfrac{k}{2\vartheta_r}(\vartheta - \vartheta_r)^2$
	heat flux/source	$\delta W_t^{\mathrm{nc}} = \dot{s}\, \delta\alpha$
dash-pot	internal dissipation	$\delta W_v^{\mathrm{nc}} = -F_v\, \delta v$

Variational Principle for Thermo-Viscoelasticity

[Maugin 2006]

$$\delta \sum_{k=0}^{N-1} \left(\int_{t_k}^{t_{k+1}} (T - \psi)\, \mathrm{d}t \right) + \sum_{k=0}^{N-1} \left(\int_{t_k}^{t_{k+1}} \delta W^{\mathrm{nc}}\, \mathrm{d}t = 0 \right)$$

dependent quantities follow from free energy ψ and internal energy U via the relations

$$\psi = U - \vartheta s \qquad U = \psi + \vartheta s$$

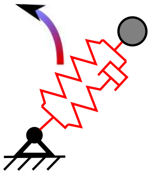
$$s = -\frac{\partial \psi}{\partial \vartheta} \qquad \vartheta = \frac{\partial U}{\partial s}$$

$$F_{ve} = \frac{\partial \psi}{\partial l}$$ total internal force

$$F_v = -\frac{\partial \psi}{\partial v}$$ viscous internal force

Thermo-viscoelastic Pendulum

[Garcia-Orden & Romero 2006]



The length of the massless pendulum rod

$$l = \sqrt{x^2 + y^2},$$

evolution equation of the dash-pot

$$\eta \dot{v} = F_v,$$

and the free energy of a thermo-elastic spring

$$\psi_e(l, \dot{\alpha}) = \frac{K}{2} \log^2\left(\frac{l}{l_0}\right) - \beta(\dot{\alpha} - \vartheta_r) \log\left(\frac{l}{l_0}\right) + k\left[\dot{\alpha} - \vartheta_r - \dot{\alpha} \log\left(\frac{\dot{\alpha}}{\vartheta_r}\right)\right].$$

Thermo-viscoelastic Pendulum

[Garcia-Orden & Romero 2006]

Free energy of the spring-damper compound (generalized Maxwell-element)

$$\psi(l, v, \vartheta) = (1+\beta_c)\psi_e + \mu v^2 - \beta_c v \frac{\partial \psi_e}{\partial l}.$$

The generalized coordinates are $\mathbf{q} = [x, y, \alpha]^T$ and their conjugated momenta

$$\begin{aligned} p_x &= \frac{\partial L}{\partial \dot{x}} = m\dot{x} \\ p_y &= \frac{\partial L}{\partial \dot{y}} = m\dot{y} \\ s &= \frac{\partial L}{\partial \dot{\alpha}} = -\frac{\partial \psi}{\partial \dot{\alpha}}. \end{aligned}$$

time derivatives are obtained from the momenta

$$\dot{x} = \frac{\partial H}{\partial x}(\mathbf{q}, \mathbf{p}), \quad \dots, \quad \dot{\alpha} = \frac{\partial U}{\partial s}(\mathbf{q}, \mathbf{p}).$$

Thermo-viscoelastic Pendulum

[Garcia-Orden & Romero 2006]

Heat transfer (Fourier type, thermal conductivity κ) between spring and environment

$$h = -\kappa(\dot{\alpha} - \vartheta_\infty).$$

Regarding the dash-pot, it is assumed that all energy mechanically dissipated is completely converted into heat, which corresponds to the entropy production

$$\dot{s}_v = \frac{g\dot{v}}{\dot{\alpha}}.$$

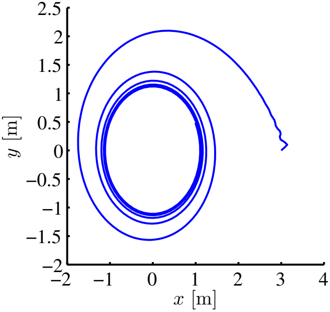
Adding the mechanical dissipation up to the previous two effects

$$\delta W^{nc} = -F_v \delta v + \frac{F_v \dot{v}}{\dot{\alpha}} \delta\alpha - \kappa \frac{\dot{\alpha} - \vartheta_\infty}{\dot{\alpha}} \delta\alpha.$$

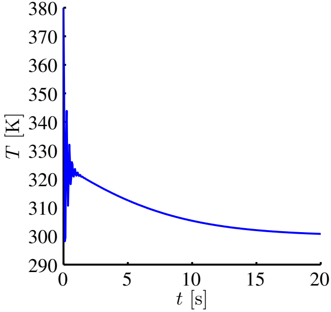
Thermo-viscoelastic Pendulum

[Garcia-Orden & Romero 2006]

free motion as example



trajectory

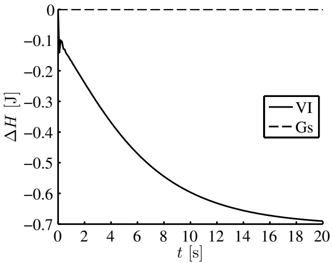


temperature

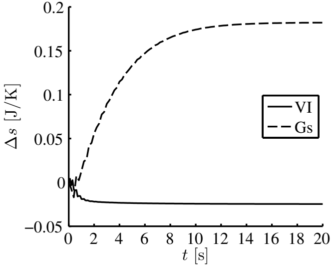
Thermo-viscoelastic Pendulum

[Garcia-Orden & Romero 2006]

comparison with energy-consistent EEM-method



energy error
$(E = 1704J)$



entropy error
$(s = 5.43 \ldots 5.46\text{J/K})$

Non-standard Heat Transfer

[Green & Naghdi 1991]

For Green & Naghdi type II heat transfer simply add

$$\psi_{\mathsf{GN2}} = \frac{1}{2}\kappa_{\mathsf{II}}|\nabla\alpha|^2$$

to the free energy.

- + Hamiltonian structure fits perfectly in VI-framework [Mata & Lew 2013]
- - low practical relevance
- - open questions

Spatial Discretization

Displacement field in a 3D-continuum element

$$\mathbf{q}(\mathbf{x}, t) = \begin{bmatrix} u(x, y, z, t) \\ v(x, y, z, t) \\ w(x, y, z, t) \end{bmatrix}$$

approximated in space first for u (v, w analogously)

$$\begin{aligned} u(x, y, z, t) &\approx \sum N^n(\mathbf{x}) u^n(t) = u^{\mathsf{sd}}(\mathbf{x}, t) \\ \dot{u}(x, y, z, t) &\approx \sum N^n(\mathbf{x}) \dot{u}^n(t) = \dot{u}^{\mathsf{sd}}(\mathbf{x}, t) \end{aligned}$$

leads as intermediate step to a semidiscrete Lagrangian

$$\begin{aligned} L &= \int_V \bar{L}(u, v, w, \dot{u}, \dot{v}, \dot{w}) \,\mathrm{d}V \\ &\approx \int_V \bar{L}(u^{\mathsf{sd}}, v^{\mathsf{sd}}, w^{\mathsf{sd}}, \dot{u}^{\mathsf{sd}}, \dot{v}^{\mathsf{sd}}, \dot{w}^{\mathsf{sd}}) \,\mathrm{d}V \\ &\approx \mathsf{I}_V^{\mathsf{num}}\Big(\bar{L}(u^{\mathsf{sd}}, \dots, \dot{w}^{\mathsf{sd}})\Big) = L_{\mathsf{sd}}\Big(\mathbf{u}(t), \dots, \dot{\mathbf{w}}(t)\Big). \end{aligned}$$

Time Discretization

Now the continous system is approximated by discrete one

$$\begin{aligned} S &= \int_{t_b}^{t_e} \int_V \bar{L}(u, v, w, \dot{u}, \dot{v}, \dot{w})\, \mathrm{d}V\, \mathrm{d}t \\ &\approx \int_0^h L_{\mathsf{sd}}(\mathbf{u}, \mathbf{v}, \mathbf{w}, \dot{\mathbf{u}}, \dot{\mathbf{v}}, \dot{\mathbf{w}})\, \mathrm{d}t = S^{\mathsf{sd}} \end{aligned}$$

VI construction as before, firstly approximation in time..

$$\mathbf{u}^d(t) = \sum_{m=0}^{p} M_m(t)\mathbf{u}_m \qquad \dot{\mathbf{u}}^d(t) = \sum_{m=0}^{p} \dot{M}_m(t)\mathbf{u}_m$$

..secondly, quadrature in time (one step)

$$\begin{aligned} S^{\mathsf{sd}} &\approx \int_0^h L_{\mathsf{sd}}(\mathbf{u}^d, \mathbf{v}^d, \mathbf{w}^d, \dot{\mathbf{u}}^d, \dot{\mathbf{v}}^d, \dot{\mathbf{w}}^d)\, \mathrm{d}t \\ &\approx \mathsf{I}_t^{\mathsf{num}}\Big(L_{\mathsf{sd}}(\mathbf{u}^d, \ldots, \dot{\mathbf{w}}^d)\Big) = L_d(\mathbf{u}_0, \mathbf{u}_1, \ldots, \mathbf{w}_p). \end{aligned}$$

Example for an Elastic Bar

spatial discretization (1 element, linear approximation)

$$\begin{aligned} L &= \frac{1}{2}\int_{-L^e/2}^{L^e/2}\left(\varrho A \dot{u}(x,t)^2 - EAu'(x,t)^2\right)\mathrm{d}x \\ &\approx \frac{1}{2}\left(\dot{\mathbf{u}}^e \cdot \mathbf{M}^e \dot{\mathbf{u}}^e - \mathbf{u}^e \cdot \mathbf{K}^e \mathbf{u}^e\right) = L_{\mathsf{sd}}\left(\mathbf{u}^e(t), \dot{\mathbf{u}}^e(t)\right) \end{aligned}$$

temporal discretization (1 time step, linear approximation)

$$\begin{aligned} \Delta S &= \int_0^h L_{\mathsf{sd}}\left(\mathbf{u}^e(t), \dot{\mathbf{u}}^e(t)\right)\mathrm{d}t \\ &\approx \frac{1}{2}\int_0^h \frac{\Delta \mathbf{u}^e}{h} \cdot \mathbf{M}^e \frac{\Delta \mathbf{u}^e}{h}\,\mathrm{d}t \\ &\quad -\frac{1}{2}\int_0^h \left(\mathbf{u}_0^e + \frac{t}{h}\Delta \mathbf{u}^e\right) \cdot \mathbf{K}^e \left(\mathbf{u}_0^e + \frac{t}{h}\Delta \mathbf{u}^e\right)\mathrm{d}t \\ &\approx \frac{h}{2}\left(\frac{\Delta \mathbf{u}^e}{h} \cdot \mathbf{M}^e \frac{\Delta \mathbf{u}^e}{h} - \frac{\mathbf{u}_0^e + \mathbf{u}_1^e}{2} \cdot \mathbf{K}^e \frac{\mathbf{u}_0^e + \mathbf{u}_1^e}{2}\right) = L_d \end{aligned}$$

Summary

Retrospect

Variational Integrators for

- discrete mechanical, conservative systems;
- with forcing and dissipation;
- with holonomic constraints.
- VIs of higher order,
- outline of thermo-mechanical coupling,
- and space-continous systems.

Outlook

- generalization to optimal control (tomorrow);
- non-smooth systems, e.g. collisions, friction;
- event-locator, adaptive time-stepping;
- electro-mechanical systems, further couplings;
- combinations of all of them, i.e. higher order VI, constrained, space-continous, coupled,...
- structure-preserving spatial discretization and model order reduction.