Variational Integrators for Thermo-Viscoelastic Discrete Systems

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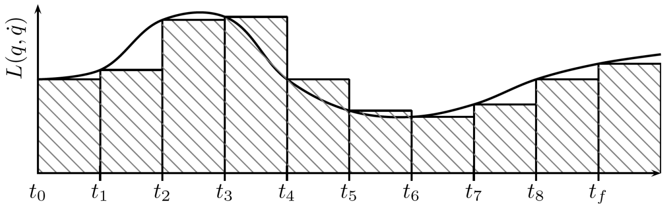
Deutsche Forschungsgemeinschaft

Introduction

Hairer, Lubich & Wanner [2012], Lew [2013], Murphey [2013]

> *"Approximate the action instead of the equations of motion"*
> A. J. Lew



[Murphey 2013]

resulting **variational integrators** offer remarkable features

- by design structure preserving (symplectic)
- excellent longtime behavior

Introduction

Hairer, Lubich & Wanner [2012], Lew [2013], Murphey [2013]

The popular Störmer-Verlet scheme is here recovered as a variational integrator for the example of a simple pendulum

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

with 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

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

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

Outline

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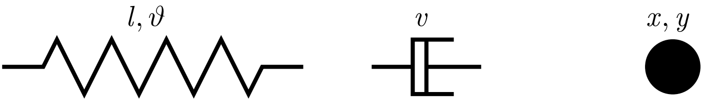
State Vector

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

Discrete Lagrangian

Marsden [2000], Ober-Blöbaum & Saake [2013]

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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

Kane et al. [1999]

..and the virtual work of the nonconservative forces

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

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

yield Discrete Euler-Lagrange-Equations
(position-momentum form)

$$\begin{aligned}
\mathbf{p}_k &= -D_1 L_d(\mathbf{q}_k, \mathbf{q}_{k+1/p} \dots, \mathbf{q}_{k+1}) - \mathbf{F}^d_k \\
\mathbf{0} &= D_2 L_d(\mathbf{q}_k, \mathbf{q}_{k+1/p} \dots, \mathbf{q}_{k+1}) + \mathbf{F}^d_{k+1/p} \\
&\dots \\
\mathbf{0} &= D_p L_d(\mathbf{q}_k, \mathbf{q}_{k+1/p} \dots, \mathbf{q}_{k+1}) + \mathbf{F}^d_{k+\frac{p-1}{p}} \\
\mathbf{p}_{k+1} &= D_{p+1} L_d(\mathbf{q}_k, \mathbf{q}_{k+1/p} \dots, \mathbf{q}_{k+1}) + \mathbf{F}^d_{k+1}
\end{aligned}$$

Variational Principle for Thermo-Viscoelasticity

Maugin [2006], Romero [2009], Bertram & Glüge [2013]

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$$\delta \int_{t_0}^{t_1} (T - \psi)\,\mathrm{d}t + \int_{t_0}^{t_1} \delta W^{\mathsf{nc}}\,\mathrm{d}t = 0$$

exemplaric expressions

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	$\delta W_t^{\mathsf{nc}} = \dot{s}\,\delta\alpha$
dash-pot	internal dissipation	$\delta W_v^{\mathsf{nc}} = F_v\,\delta v$

Variational Principle for Thermo-Viscoelasticity

Maugin [2006], Romero [2009], Bertram & Glüge [2013]

$$\delta \int_{t_0}^{t_1} (T - \psi)\, \mathrm{d}t + \int_{t_0}^{t_1} \delta W^{\mathrm{nc}}\, \mathrm{d}t = 0$$

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

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

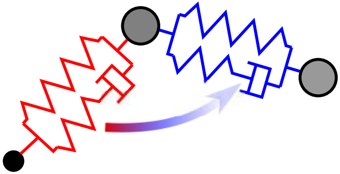
$$s = -\frac{\partial \psi}{\partial \vartheta} \qquad \vartheta = \frac{\partial U}{\partial s}$$

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

$$F_{v} = -\frac{\partial \psi}{\partial v} \qquad \text{viscous internal force}$$

Thermoviscoelastic Double Pendulum

Romero [2009], Krüger & Groß & Betsch [2010], Conde [2015]



two concentrated masses connected by thermoviscoelastic springs with heat conduction between them

Lagrangian $L = T - \psi$

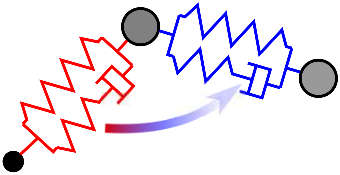
$$T = \sum_{i=1}^{2} \frac{1}{2} m_i (\dot{x}_i^2 + \dot{y}_i^2)$$

$$\psi = \sum_{j=1}^{2} (1+\gamma_j)\psi_j^\infty + \mu_j v_j^2 - \gamma_j \frac{\partial \psi_j^\infty}{\partial l_j}$$

$$\psi^\infty = \frac{1}{2} K \log^2 \frac{l}{l_0} - \beta \Delta\vartheta \log \frac{l}{l_0} + k \left(\Delta\vartheta - \vartheta \log \frac{\vartheta}{\vartheta_r} \right)$$

Thermoviscoelastic Double Pendulum

Romero [2009], Krüger & Groß & Betsch [2010], Conde [2015]



two concentrated masses connected by thermoviscoelastic springs with heat conduction between them

virtual work of heat transfer (Fourier Type) and viscosity

$$\delta W^{nc} = \kappa \frac{\dot{\alpha}_2 - \dot{\alpha}_1}{\dot{\alpha}_1} \delta\alpha_1 + \kappa \frac{\dot{\alpha}_1 - \dot{\alpha}_2}{\dot{\alpha}_2} \delta\alpha_2 - \sum_{j=1}^{2} F_{vj}\, \delta v_j + \sum_{j=1}^{2} \frac{F_{vj}\, \dot{v}_j}{\dot{\alpha}_j} \delta\alpha_j$$

further assumed linear viscosity (internal variable v)

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

Time Stepping Scheme I

Dominik Kern[1], Ignacio Romero[2], Michael Groß[1]

classical formulation

equations of motion

$$
\begin{aligned}
m\ddot{x}_1 &+ \left(\frac{\partial\psi}{\partial l_1}\frac{x_1}{l_1} - \frac{\partial\psi}{\partial l_2}\frac{(x_2-x_1)}{l_2}\right) &&= F_{1x}\\
m\ddot{y}_1 &+ \left(\frac{\partial\psi}{\partial l_1}\frac{y_1}{l_1} - \frac{\partial\psi}{\partial l_2}\frac{(y_2-y_1)}{l_2}\right) &&= F_{1y}\\
m\ddot{x}_2 &+ \frac{\partial\psi}{\partial l_2}\frac{(x_2-x_1)}{l_2} &&= F_{2x}\\
m\ddot{y}_2 &+ \frac{\partial\psi}{\partial l_2}\frac{(y_2-y_1)}{l_2} &&= F_{2y}\\
\frac{k_1}{\dot{\alpha}_1}\ddot{\alpha}_1 &+ \beta_1\frac{x_1\dot{x}_1 + y_1\dot{y}_1}{l_1^2} &&= \dot{s}_1\\
\frac{k_2}{\dot{\alpha}_2}\ddot{\alpha}_2 &+ \beta_2\frac{(x_2-x_1)(\dot{x}_2-\dot{x}_1)+(y_2-y_1)(\dot{y}_2-\dot{y}_1)}{l_2^2} &&= \dot{s}_2
\end{aligned}
$$

evolution equations

$$
\begin{aligned}
\eta\dot{v}_1 &= \frac{\partial\psi}{\partial v_1}\\
\eta\dot{v}_2 &= \frac{\partial\psi}{\partial v_2}
\end{aligned}
$$

Dominik Kern[1], Ignacio Romero[2], Michael Groß[1]

Time Stepping Scheme II

$$\begin{aligned} \mathbf{p}_0 &= -D_1 L_d - \mathbf{F}_0^d \\ \mathbf{0} &= D_2 L_d + \mathbf{F}_{1/2}^d \\ \mathbf{p}_1 &= D_3 L_d + \mathbf{F}_1^d \end{aligned}$$

$$\begin{aligned} D_1 L_d &= \frac{\partial L_d}{\mathbf{q}_0} \\ &= \sum_{j=1}^{g} w_m \left(\frac{\partial T}{\mathbf{q}_0} - \frac{\partial \psi}{\mathbf{q}_0} \right)_{t=t_m} \\ &= \sum_{j=1}^{g} w_m \left(\begin{bmatrix} m\dot{x}_1 \\ m\dot{y}_1 \\ -\frac{\partial \psi}{\partial \dot{\alpha}_1} \\ 0 \\ \dots \end{bmatrix} \frac{\partial \dot{q}^d}{\partial q_0} + \begin{bmatrix} -\frac{\partial \psi}{\partial l_1}\frac{\partial l_1}{\partial x_1} \\ -\frac{\partial \psi}{\partial l_1}\frac{\partial l_1}{\partial y_1} \\ 0 \\ -\frac{\partial \psi}{\partial v_1} \\ \dots \end{bmatrix} \frac{\partial q^d}{\partial q_0} \right)_{t=t_m} \end{aligned}$$

with $\frac{\partial q^d}{\partial q_0} = \frac{2t^2}{h} - \frac{3t}{h} + 1$ and $\frac{\partial \dot{q}^d}{\partial q_0} = \frac{4t}{h^2} - \frac{3}{h}$

Time Stepping Scheme III

Dominik Kern[1], Ignacio Romero[2], Michael Groß[1]

$$
\begin{aligned}
\mathbf{p}_0 &= -D_1 L_d - \mathbf{F}_0^d \\
\mathbf{0} &= D_2 L_d + \mathbf{F}_{1/2}^d \\
\mathbf{p}_1 &= D_3 L_d + \mathbf{F}_1^d
\end{aligned}
$$

$$
\begin{aligned}
F_0^d &= \frac{\partial}{\mathbf{q}_0} \delta W_d^{nc} \\
&= \sum_{j=1}^{g} w_m \left(\frac{\partial}{\partial \mathbf{q}_0} \mathbf{F} \cdot \delta \mathbf{q} \right)_{t=t_m} \\
&= \sum_{j=1}^{g} w_m \left(\begin{bmatrix} F_{1x} \\ F_{1y} \\ \dot{s}_1 \\ F_{1v} \\ \dots \end{bmatrix} \frac{\partial q^d}{\partial q_0} \right)_{t=t_m}
\end{aligned}
$$

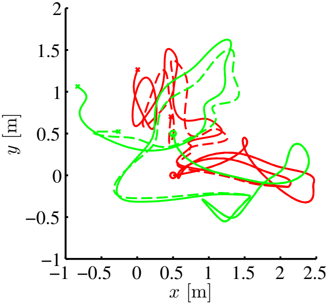
with $\frac{\partial q^d}{\partial q_0} = \frac{2t^2}{h} - \frac{3t}{h} + 1$ and $\frac{\partial \dot{q}^d}{\partial q_0} = \frac{4t}{h^2} - \frac{3}{h}$

Results I

quadratic approximation (Lagrange polynomials) using

- Gauss-Lobatto quadrature of 2.order (L2GLo2)
- Gauss-Lobatto quadrature of 5.order (L2GLo5)

animation



trajectories

Results II

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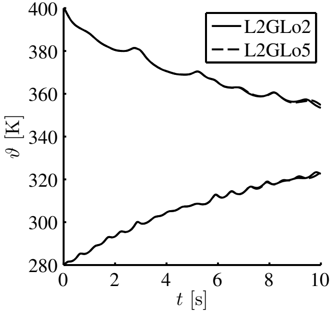
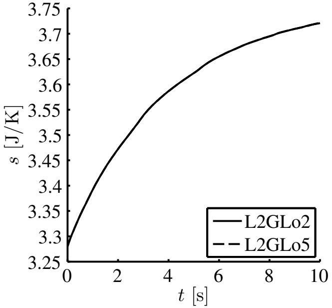


temperatures



entropy

Results III

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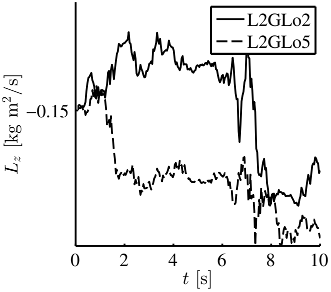
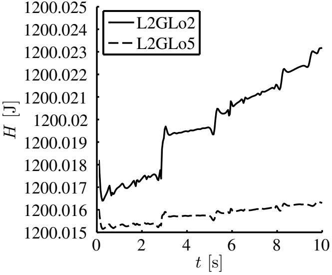
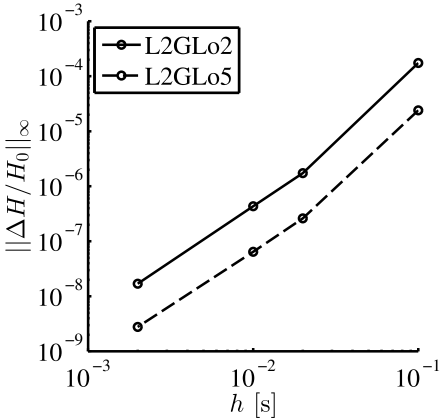


angular momentum



total energy

Results IV



relative error in total energy vs time step for VI with Gauss-Lobatto quadrature of 2. and 5.order, both using quadratic approximation (Lagrange polynomials of 2.order)

Fourier Heat Transfer vs. Green & Naghdi type II

Green & Naghdi [1991], Bargmann [2013], Mata & Lew [2014]

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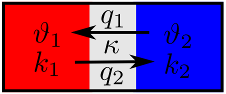


thermal only: two heat reservoirs connected by a channel

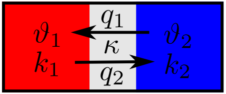
motivation: modeling of second sound and
demonstrate conservation properties of VI

$$\psi_{\mathsf{GN}} = \underbrace{k\left(\vartheta - \vartheta_r - \vartheta \log\frac{\vartheta}{\vartheta_r}\right)}_{\psi_{\text{standard}}} + \frac{1}{2}\frac{\kappa_{II}}{\vartheta_r}(\underbrace{\alpha_2 - \alpha_1}_{\text{“gradient”}})^2$$

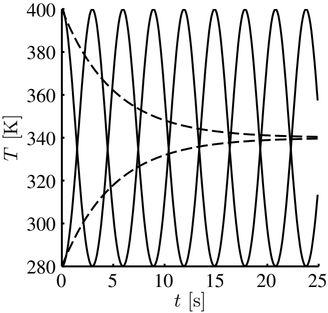
$$\dot{\mathbf{s}}_{\mathsf{GN}} = -\frac{\kappa_{II}}{\vartheta_r}(\alpha_2 - \alpha_1)$$

Fourier Heat Transfer vs. Green & Naghdi type II

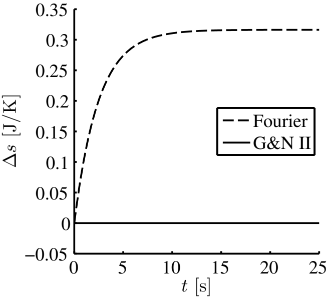
Green & Naghdi [1991], Bargmann [2013], Mata & Lew [2014]



thermal only: two heat reservoirs connected by a channel

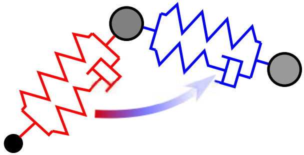


temperatures

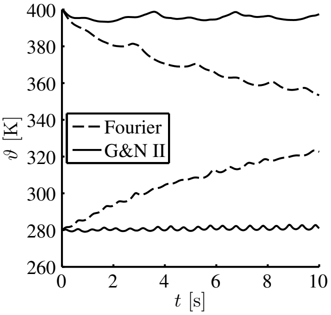


entropy

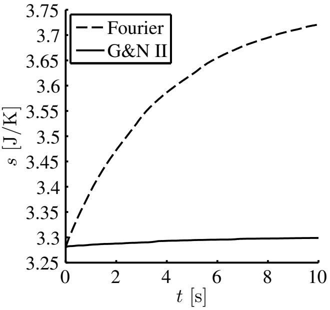
Fourier vs. Green & Naghdi type II



double pendulum with heat conduction



temperatures



entropy

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Summary and Outlook

An existing variational time integrator for finite-dimensional thermo-elasto-dynamics with heat conduction was enhanced by the inclusion of viscosity and non-standard heat transfer.

- good conservation properties
- quadrature of higher order than approximation seems not to improve convergence

Future work is related with

- combine explicit and implicit schemes within one VI
- constraints and control actions

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DFG Deutsche Forschungsgemeinschaft

Simulation Parameters

h	0.1	s
$m_1 = m_2$	1	kg
$K_1 = K_2$	10	J
$l_{0,1} = l_{0,2}$	0.5	m
$\beta_1 = \beta_2$	0.1	J/K
$\gamma_1 = \gamma_2$	0.5	–
$\eta_1 = \eta_2$	10	Ns/m
$\mu_1 = \mu_2$	1	N/m
$k_1 = k_2$	10	J/K
κ	1	W/K
κ_{II}	5	W/Ks
ϑ_r	300	K

double pendulum model parameters

Simulation Parameters

$x_1(0)$	0.5	m
$y_1(0)$	0	m
$\dot{x}_1(0)$	0	m/s
$\dot{y}_1(0)$	-0.1	m/s
$v_1(0)$	0	m
$\alpha_1(0)$	0	Ks
$\vartheta_1(0)$	400	K

$x_2(0)$	0.5	m
$y_2(0)$	0.5	m
$\dot{x}_2(0)$	0.1	m/s
$\dot{y}_2(0)$	-0.1	m/s
$v_2(0)$	0	m
$\alpha_2(0)$	0	Ks
$\vartheta_2(0)$	280	K

double pendulum initial conditions

Simulation Parameters

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$k_1 = k_2$	10	J/K
κ	1	W/K
κ_{II}	5	W/Ks
ϑ_r	300 K	
$\alpha_1(0)$	0	Ks
$\vartheta_1(0)$	400	K
$\alpha_2(0)$	0	Ks
$\vartheta_2(0)$	280	K

thermal only model