Variational Integrators for Thermomechanical Coupled Dynamic Systems with Heat Conduction

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March 11, 2014

GAMM 2014
S1: Multibody Dynamics
Example
Romero [2009], Krüger & Groß & Betsch [2010]

thermoelastic double pendulum
- free motion of two discrete masses connected by thermoelastic springs
- adiabatic system, heat transfer only between springs
Variational Integrators

"Variational methods turn out to be not only esthetically and logically most satisfactory, but at the same time very practical by providing a tool for the solution of many dynamical problems."

C. Lanczos

\[ \delta S = \delta \int_{t_0}^{t_1} L(z, \dot{z}) \, dt = 0 \]

time discretization

\[ z(t) \approx z^h(t, z^k, z^{k+1}) \]

discrete Langrangian

\[ L_d(z^k, z^{k+1}) = \int_{t^k}^{t^{k+1}} L(z^h(t), \dot{z}^h(t)) \, dt \]

discrete action sum

\[ S_d = (z^0, \ldots, z^N) = \sum_{k=0}^{N-1} L_d(z^k, z^{k+1}) \]

advantages:

- by design structure preserving (symplectic)
- excellent longtime behavior
“The variational characterization of the thermoelastic problem means the identification of a functional whose stationary points are solutions of the problem.”

G. Maugin

\[ S = \int_{t_0}^{t_1} L \, dt \]

\[ L = T(x, v) - \Psi(F, \Phi, \vartheta, \gamma) \]
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Thermoelasticity

Maugin [2006], Gross & Betsch [2011], Romero [2011]

\begin{align*}
\text{mechanical} & \quad \text{thermal} \\
\text{deformation} & \quad x = x(X, t) & \quad \text{thermacy} & \quad \Phi = \Phi(X, t) \\
\text{mapping} & \quad \text{velocity} & \quad \mathbf{v} = \dot{x} & \quad \text{temperature} & \quad \vartheta = \dot{\Phi} \\
\text{deformation} & \quad \mathbf{F} = \nabla_x \mathbf{x} & \quad \text{thermal gradient} & \quad \mathbf{\gamma} = \nabla_x \Phi \\
\text{gradient} & \quad \text{momentum} & \quad p = \frac{\partial L}{\partial \mathbf{v}} & \quad \text{entropy} & \quad \eta = \frac{\partial L}{\partial \vartheta}
\end{align*}

Green and Naghdi type II
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Outline

1. Introduction

2. Variational Integrator by Generalized Trapezoidal Rule

3. Thermoelastic Double Pendulum as Model Problem

4. Verification

5. Summary and Outlook
Discrete Lagrangian (GTR)

linear interpolation by generalized trapezoidal rule (GTR)

\[ L_d(z^k, z^{k+1}) = \Delta t \left\{ \alpha L(z(t^k), \dot{z}(t^k)) + (1 - \alpha) L(z(t^{k+1}), \dot{z}(t^{k+1})) \right\} \]

discrete Euler-Lagrange equations

\[ 0 = D_2 L_d(z^{k-1}, z^k) + D_1 L_d(z^k, z^{k+1}) \]

with (using GTR)

\[ D_1 L_d(z^k, z^{k+1}) = \alpha \frac{\partial L}{\partial z^k} \Delta t + \frac{\partial L}{\partial \dot{z}^{k+1}} \]

\[ D_2 L_d(z^{k-1}, z^k) = (1 - \alpha) \frac{\partial L}{\partial z^k} \Delta t + \frac{\partial L}{\partial \dot{z}^k} \]
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Forced Discrete Lagrange-D’Alembert-Principle

\[ 0 = \sum_{k=0}^{N} \delta L_d(z^k, z^{k+1}) + \sum_{k=0}^{N} \delta W_d(z^k, z^{k+1}) \]

\[ = \sum_{k=0}^{N} \delta L_d(z^k, z^{k+1}) + \sum_{k=0}^{N} \int_{t^k}^{t^{k+1}} f_d(z(\tau)) \delta z(\tau) \, d\tau \]

position-momentum form

\[ \Pi^k = -D_1 L_d(z^k, z^{k+1}) - f_d^- \]

\[ \Pi^{k+1} = D_2 L_d(z^k, z^{k+1}) + f_d^+ \]

discrete generalized forces (mechanical forces, entropy flux)

\[ f_d^- = \int_{t^k}^{t^{k+1}} f_d(\tau) \frac{\partial z(\tau)}{\partial z^k} \, d\tau = \Delta t \, \alpha \, f_d(t^k) \]

\[ f_d^+ = \int_{t^k}^{t^{k+1}} f_d(\tau) \frac{\partial z(\tau)}{\partial z^{k+1}} \, d\tau = \Delta t \, (1 - \alpha) \, f_d(t^{k+1}) \]


Higher Order Integrators

\[ L_d(z^k, z^{k+1/2}, z^{k+1}) \frac{6}{\Delta t} = \]

\[ \sum_{i=1}^{2} \frac{1}{2} m_i \left\{ (v_i^k)^T v_i^k + 4(v_i^{k+1/2})^T v_i^{k+1/2} + (v_i^{k+1})^T v_i^{k+1} \right\} \]

\[ - \sum_{j=1}^{2} \left\{ \psi_j(c_j^k, \vartheta_j^k) + 4\psi_j(c_j^{k+1/2}, \vartheta_j^{k+1/2}) + \psi_j(c_j^{k+1}, \vartheta_j^{k+1}) \right\} \]
Thermoelastic Double Pendulum

Romero [2009], Krüger & Groß & Betsch [2010], Krüger [2013]

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model of mechanical system: two concentrated masses connected by elastic springs

defformation measure

\[ c_1 = \lambda_1^2 = \left( \frac{l_1}{l_0^1} \right)^2 = \frac{r_1^T r_1}{r_0^T r_0} \]

\[ c_2 = \lambda_2^2 = \left( \frac{l_2}{l_0^2} \right)^2 = \frac{(r_2 - r_1)^T (r_2 - r_1)}{(r_2^0 - r_1^0)^T (r_2^0 - r_1^0)} \]
model of thermal system: two heat reservoirs connected by a heat channel

Fourier’s law

\[ q_1 = -\kappa (\vartheta_1 - \vartheta_2) \]
\[ q_2 = -q_1 \]
Thermoelastic Double Pendulum

Simo [1995]

Free energy function of the spring \( j = \{1, 2\} \)

\[
\psi_j = \psi_{\text{mech}}(c_j) + \psi_{\text{coupled}}(c_j, \vartheta_j) + \psi_{\text{thermal}}(\vartheta_j)
\]

\[
\psi_{\text{mech}} = \frac{K_j}{2} \log^2 \left( \frac{c_j^{1/2}}{2} \right)
\]

\[
\psi_{\text{coupled}} = \frac{\beta_j}{2} (\vartheta_\infty - \vartheta_j) \log \left( \frac{c_j^{1/2}}{2} \right)
\]

\[
\psi_{\text{thermal}} = k_j \left[ \vartheta_j - \vartheta_\infty - \vartheta_j \log \left( \frac{\vartheta_j}{\vartheta_\infty} \right) \right]
\]

- \( K_j \) spring stiffness
- \( \beta_j \) thermomechanical coupling parameter
- \( k_j \) heat capacity
Double Pendulum – Discretization

Lagrange function

\[ L(z, \dot{z}) = \frac{1}{2} \sum_{i=1}^{2} m_i |\dot{r}_i|^2 - \psi_1(c_1, \dot{\Phi}_1) - \psi_2(c_2, \dot{\Phi}_2) \]

Discrete Lagrangian (GTR) with \( z = [r_1, r_2, \Phi_1, \Phi_2]^T \)

\[ \frac{L_d(z^k, z^{k+1})}{\Delta t} = \frac{1}{2} \sum_{i=1}^{2} \alpha m_i |\dot{r}_i^k|^2 + (1 - \alpha) m_i |\dot{r}_i^{k+1}|^2 \]

\[ - \sum_{j=1}^{2} \alpha \psi_j(c_j^k, \dot{\Phi}_j^k) + (1 - \alpha) \psi_j(c_j^{k+1}, \dot{\Phi}_j^{k+1}) \]

\[ \dot{r}_i^k = \dot{r}_i^{k+1} = \frac{r_i^{k+1} - r_i^k}{\Delta t} \]

\[ \dot{\Phi}_j^k = \dot{\Phi}_j^{k+1} = \frac{\Phi_j^{k+1} - \Phi_j^k}{\Delta t} \]
Double Pendulum – Discretization

position-momentum form – mechanical equations

\[ p_i^k = m_i \frac{r_i^{k+1} - r_i^k}{\Delta t} + \alpha \Delta t \sum_{j=1}^{2} D_1 \psi_j(c_j^k, \vartheta_j^k) \frac{\partial c_j^k}{\partial r_i^k} \]

\[ p_i^{k+1} = m_i \frac{r_i^{k+1} - r_i^k}{\Delta t} \]

\[ -(1 - \alpha) \Delta t \sum_{j=1}^{2} D_1 \psi_j(c_j^{k+1}, \vartheta_j^{k+1}) \frac{\partial c_j^{k+1}}{\partial r_i^{k+1}} \]

\[ c_1 = \frac{r_1^T r_1}{r_1^T r_1} \]

\[ c_2 = \frac{(r_2 - r_1)^T (r_2 - r_1)}{(r_2^0 - r_1^0)^T (r_2^0 - r_1^0)} \]

\[ \vartheta_j = \dot{\Phi}_j \]
Double Pendulum – Discretization

position-momentum form – thermal equations

\[ \eta_j^k = - \left\{ \alpha D_2 \psi_j(c_j^k, \vartheta_j^k) + (1 - \alpha) D_2 \psi_j(c_j^{k+1}, \vartheta_j^{k+1}) \right\} \]
\[ - \alpha \Delta t f_{thj}^k \]
\[ \eta_j^{k+1} = - \left\{ \alpha D_2 \psi_j(c_j^k, \vartheta_j^k) + (1 - \alpha) D_2 \psi_j(c_j^{k+1}, \vartheta_j^{k+1}) \right\} \]
\[ + (1 - \alpha) \Delta t f_{thj}^{k+1} \]

\[ f_{thj}^k = \frac{q_j^k}{\vartheta_j^k} \]
\[ f_{thj}^{k+1} = \frac{q_j^{k+1}}{\vartheta_j^{k+1}} \]
Double Pendulum – Discretization

\[ p_i^{k+1} = m_i \frac{r_i^{k+1} - r_i^k}{\Delta t} + \alpha \Delta t \sum_{j=1}^{2} D_1 \psi_j(c_j^k, \vartheta_j^k) \frac{\partial c_j^k}{\partial r_i^k} \]

\[ \eta_j^k = - \left\{ \alpha D_2 \psi_j(c_j^k, \vartheta_j^k) + (1 - \alpha) D_2 \psi_j(c_j^{k+1}, \vartheta_j^{k+1}) \right\} \]

\[ -\alpha \Delta t \frac{q_j^k}{\vartheta_j^k} \]

\[ p_i^k = m_i \frac{r_i^{k+1} - r_i^k}{\Delta t} \]

\[ -(1 - \alpha) \Delta t \sum_{j=1}^{2} D_1 \psi_j(c_j^{k+1}, \vartheta_j^{k+1}) \frac{\partial c_j^{k+1}}{\partial r_i^{k+1}} \]

\[ \eta_j^{k+1} = - \left\{ \alpha D_2 \psi_j(c_j^k, \vartheta_j^k) + (1 - \alpha) D_2 \psi_j(c_j^{k+1}, \vartheta_j^{k+1}) \right\} \]

\[ +(1 - \alpha) \Delta t \frac{q_j^{k+1}}{\vartheta_j^{k+1}} \]
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Double Pendulum – Digest

- variational formulation \( L = T - \Psi \)
- time discretization \( z^k \)
- discrete Lagrangian \( L_d \)
- discrete action sum \( S_d \)
- position-momentum form
  - iterative solution: \( p_i^k, \eta_j^k \) \( \leadsto \) \( r_i^{k+1}, \Phi_j^{k+1} \)
  - update equation: \( r_i^{k+1}, \Phi_j^{k+1} \) \( \leadsto \) \( p_i^{k+1}, \eta_j^{k+1} \)
Special Cases – Thermal only

analytical and numerical (VI-GTR, $\alpha = 0.5$) solution
Special Cases – Thermal only

difference between numerical (VI-GTR, \( \alpha = 0.5 \)) and analytical solution (\( H = 800.015 \))
Special Cases – Thermal only

analytical and numerical (VI-GTR, $\alpha = 0.5$) solution
analytical and numerical (VI-GTR, $\alpha = 0.5$) solution for small displacements in $y$-direction only
Reference Results


comparison between different integrators
Reference Results

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Comparison between different integrators
Comparison of different $\alpha$-values of the VI-GTR integrator.
Reference Results

comparison of different $\alpha$-values of the VI-GTR integrator
An existing variational time integrator for finite-dimensional thermo-elasto-dynamics was enhanced by the inclusion of heat conduction. Its results are in accordance with

- the second law of thermodynamics,
- analytical solutions for special cases,
- reference solutions from the literature for general cases.

Future work is related with

- reformulation of the heat transfer in potential-like functions (nonstandard heat transfer),
- extension to viscoelasticity and plasticity,
- dissipation by fluid-structure interaction,
- extension to general discrete systems (MBS),
- extension to flexible bodies (flexMBS).