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

Marsden [2001], Zielonka [2006], Leyendecker & Marsden & Ortiz [2008], Mata & Lew [2011]

> *"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

$$\delta S = \delta \int_{t_0}^{t_1} L(\mathbf{z}, \dot{\mathbf{z}})\,\mathrm{d}t = 0$$

time discretization $\quad \mathbf{z}(t) \approx \mathbf{z}^h(t, \mathbf{z}^k, \mathbf{z}^{k+1})$

discrete Langrangian $\quad L_d(\mathbf{z}^k, \mathbf{z}^{k+1}) = \int_{t^k}^{t^{k+1}} L(\mathbf{z}^h(t), \dot{\mathbf{z}}^h(t))\,\mathrm{d}t$

discrete action sum $\quad S_d = (\mathbf{z}^0, \dots, \mathbf{z}^N) = \sum_{k=0}^{N-1} L_d(\mathbf{z}^k, \mathbf{z}^{k+1})$

advantages:

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

Thermoelasticity

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

> *"The variational characterization of the thermoelastic problem means the identification of a functional whose stationary points are solutions of the problem."*
>
> G. Maugin

$$
\begin{aligned}
S &= \int_{t_0}^{t_1} L \,\mathrm{d}t \\
L &= T(\mathbf{x}, \mathbf{v}) - \Psi(\mathbf{F}, \Phi, \vartheta, \boldsymbol{\gamma})
\end{aligned}
$$

Thermoelasticity

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

mechanical		thermal	
deformation mapping	$\mathbf{x} = \mathbf{x}(\mathbf{X}, t)$	thermacy	$\Phi = \Phi(\mathbf{X}, t)$
velocity	$\mathbf{v} = \dot{\mathbf{x}}$	temperature	$\vartheta = \dot{\Phi}$
deformation gradient	$\mathbf{F} = \nabla_X \mathbf{x}$	thermal gradient	$\boldsymbol{\gamma} = \nabla_X \Phi$
momentum	$\mathbf{p} = \frac{\partial L}{\partial \mathbf{v}}$	entropy	$\eta = \frac{\partial L}{\partial \vartheta}$

Green and Naghdi type II

Outline

Discrete Lagrangian (GTR)

linear interpolation by generalized trapezoidal rule (GTR)

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

discrete Euler-Lagrange equations

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

with (using GTR)

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

$$D_2 L_d(\mathbf{z}^{k-1}, \mathbf{z}^k) = (1-\alpha) \frac{\partial L}{\partial \mathbf{z}^k} \Delta t + \frac{\partial L}{\partial \dot{\mathbf{z}}^k}$$

Forced Discrete Lagrange-D'Alembert-Principle

$$\begin{aligned} 0 &= \sum_{k=0}^{N} \delta L_d(\mathbf{z}^k, \mathbf{z}^{k+1}) + \sum_{k=0}^{N} \delta W_d(\mathbf{z}^k, \mathbf{z}^{k+1}) \\ &= \sum_{k=0}^{N} \delta L_d(\mathbf{z}^k, \mathbf{z}^{k+1}) + \sum_{k=0}^{N} \int_{t^k}^{t^{k+1}} \mathbf{f}_d(\mathbf{z}(\tau)) \delta \mathbf{z}(\tau)\, \mathrm{d}t \end{aligned}$$

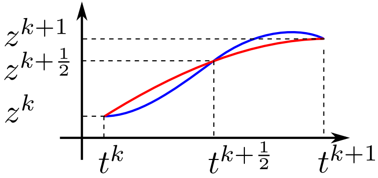
position-momentum form

$$\begin{aligned} \mathbf{\Pi}^k &= -D_1 L_d(\mathbf{z}^k, \mathbf{z}^{k+1}) - \mathbf{f}_d^- \\ \mathbf{\Pi}^{k+1} &= D_2 L_d(\mathbf{z}^k, \mathbf{z}^{k+1}) + \mathbf{f}_d^+ \end{aligned}$$

discrete generalized forces (mechanical forces, entropy flux)

$$\begin{aligned} \mathbf{f}_d^- &= \int_{t^k}^{t^{k+1}} \mathbf{f}_d(\tau) \frac{\partial \mathbf{z}(\tau)}{\partial \mathbf{z}^k} d\tau = \Delta t\ \alpha\ \mathbf{f}_d(t^k) \\ \mathbf{f}_d^+ &= \int_{t^k}^{t^{k+1}} \mathbf{f}_d(\tau) \frac{\partial \mathbf{z}(\tau)}{\partial \mathbf{z}^{k+1}} d\tau = \Delta t\ (1-\alpha)\ \mathbf{f}_d(t^{k+1}) \end{aligned}$$

Higher Order Integrators

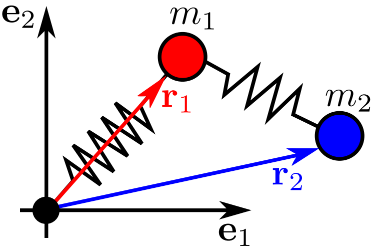


quadratic interpolation

$$L_d(\mathbf{z}^k, \mathbf{z}^{k+1/2}, \mathbf{z}^{k+1}) \frac{6}{\Delta t} =$$
$$\textstyle\sum_{i=1}^{2} \frac{1}{2} m_i \left\{ (\mathbf{v}_i^k)^T \mathbf{v}_i^k + 4(\mathbf{v}_i^{k+1/2})^T \mathbf{v}_i^{k+1/2} + (\mathbf{v}_i^{k+1})^T \, \mathbf{v}_i^{k+1} \right\}$$
$$- \textstyle\sum_{j=1}^{2} \left\{ \psi_j(c_j^k, \vartheta_j^k) + 4\psi_j(c_j^{k+1/2}, \vartheta_j^{k+1/2}) + \psi_j(c_j^{k+1}, \vartheta_j^{k+1}) \right\}$$

Thermoelastic Double Pendulum

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



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

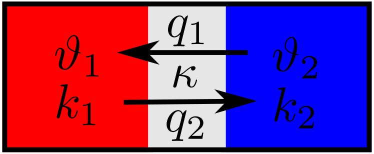
deformation measure

$$c_1 = \lambda_1^2 = \left(\frac{l_1}{l_1^0}\right)^2 = \frac{\mathbf{r}_1^T \mathbf{r}_1}{\mathbf{r}_1^{0\,T} \mathbf{r}_1^0}$$

$$c_2 = \lambda_2^2 = \left(\frac{l_2}{l_2^0}\right)^2 = \frac{(\mathbf{r}_2 - \mathbf{r}_1)^T (\mathbf{r}_2 - \mathbf{r}_1)}{(\mathbf{r}_2^0 - \mathbf{r}_1^0)^T (\mathbf{r}_2^0 - \mathbf{r}_1^0)}$$

Thermoelastic Double Pendulum

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



model of thermal system: two heat reservoirs connected by a heat channel

Fourier's law

$$q_1 = -\kappa\left(\vartheta_1 - \vartheta_2\right)$$
$$q_2 = -q_1$$

Thermoelastic Double Pendulum

Simo [1995]

free energy function of the spring $j = \{1, 2\}$

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

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

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

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

K_j	spring stiffness
β_j	thermomechanical coupling parameter
k_j	heat capacity

Double Pendulum – Discretization

Lagrange function

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

Discrete Lagrangian (GTR) with $\mathbf{z} = [\mathbf{r}_1, \mathbf{r}_2, \Phi_1, \Phi_2]^T$

$$\frac{L_d(\mathbf{z}^k, \mathbf{z}^{k+1})}{\Delta t} = \frac{1}{2} \sum_{i=1}^{2} \alpha m_i |\dot{\mathbf{r}}_i^k|^2 + (1-\alpha) m_i |\dot{\mathbf{r}}_i^{k+1}|^2 - \sum_{j=1}^{2} \alpha \psi_j(c_j^k, \dot{\Phi}_j^k) + (1-\alpha)\psi_j(c_j^{k+1}, \dot{\Phi}_j^{k+1})$$

$$\dot{\mathbf{r}}_i^k = \dot{\mathbf{r}}_i^{k+1} = \frac{\mathbf{r}_i^{k+1} - \mathbf{r}_i^k}{\Delta t} \qquad \dot{\Phi}_j^k = \dot{\Phi}_j^{k+1} = \frac{\Phi_j^{k+1} - \Phi_j^k}{\Delta t}$$

Double Pendulum – Discretization

position-momentum form – mechanical equations

$$
\begin{aligned}
\mathbf{p}_i^k &= m_i \frac{\mathbf{r}_i^{k+1} - \mathbf{r}_i^k}{\Delta t} + \alpha \Delta t \sum_{j=1}^{2} D_1 \psi_j(c_j^k, \vartheta_j^k) \frac{\partial c_j^k}{\partial \mathbf{r}_i^k} \\
\mathbf{p}_i^{k+1} &= m_i \frac{\mathbf{r}_i^{k+1} - \mathbf{r}_i^k}{\Delta t} \\
&\quad - (1-\alpha)\Delta t \sum_{j=1}^{2} D_1 \psi_j(c_j^{k+1}, \vartheta_j^{k+1}) \frac{\partial c_j^{k+1}}{\partial \mathbf{r}_i^{k+1}}
\end{aligned}
$$

$$c_1 = \frac{\mathbf{r}_1^T \mathbf{r}_1}{\mathbf{r}_1^{0\,T} \mathbf{r}_1^0} \qquad c_2 = \frac{(\mathbf{r}_2 - \mathbf{r}_1)^T (\mathbf{r}_2 - \mathbf{r}_1)}{(\mathbf{r}_2^0 - \mathbf{r}_1^0)^T (\mathbf{r}_2^0 - \mathbf{r}_1^0)} \qquad \vartheta_j = \dot{\Phi}_j$$

Double Pendulum – Discretization

position-momentum form – thermal equations

$$\begin{aligned}\eta_j^k &= -\left\{\alpha D_2\psi_j(c_j^k,\vartheta_j^k) + (1-\alpha)D_2\psi_j(c_j^{k+1},\vartheta_j^{k+1})\right\}\\ &\quad -\alpha\ \Delta t\, f_{th_j}^k\\ \eta_j^{k+1} &= -\left\{\alpha D_2\psi_j(c_j^k,\vartheta_j^k) + (1-\alpha)D_2\psi_j(c_j^{k+1},\vartheta_j^{k+1})\right\}\\ &\quad +(1-\alpha)\ \Delta t\, f_{th_j}^{k+1}\end{aligned}$$

$$f_{th_j}^k = \frac{q_j^k}{\vartheta_j^k} \qquad f_{th_j}^{k+1} = \frac{q_j^{k+1}}{\vartheta_j^{k+1}}$$

Double Pendulum – Discretization

$$\mathbf{p}_i^k = m_i \frac{\mathbf{r}_i^{k+1} - \mathbf{r}_i^k}{\Delta t} + \alpha \Delta t \sum_{j=1}^{2} D_1 \psi_j(c_j^k, \vartheta_j^k) \frac{\partial c_j^k}{\partial \mathbf{r}_i^k}$$

$$\eta_j^k = -\left\{\alpha D_2 \psi_j(c_j^k, \vartheta_j^k) + (1-\alpha) D_2 \psi_j(c_j^{k+1}, \vartheta_j^{k+1})\right\} - \alpha \; \Delta t \, \frac{q_j^k}{\vartheta_j^k}$$

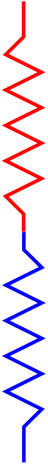
$$\mathbf{p}_i^{k+1} = m_i \frac{\mathbf{r}_i^{k+1} - \mathbf{r}_i^k}{\Delta t} - (1-\alpha) \Delta t \sum_{j=1}^{2} D_1 \psi_j(c_j^{k+1}, \vartheta_j^{k+1}) \frac{\partial c_j^{k+1}}{\partial \mathbf{r}_i^{k+1}}$$

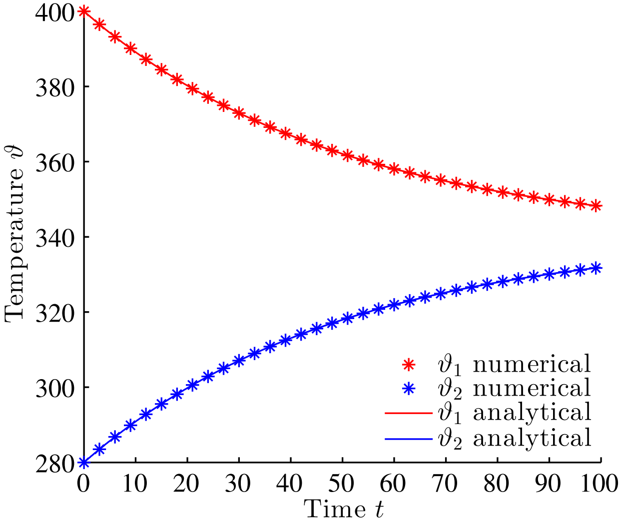
$$\eta_j^{k+1} = -\left\{\alpha D_2 \psi_j(c_j^k, \vartheta_j^k) + (1-\alpha) D_2 \psi_j(c_j^{k+1}, \vartheta_j^{k+1})\right\} + (1-\alpha) \; \Delta t \, \frac{q_j^{k+1}}{\vartheta_j^{k+1}}$$

Double Pendulum – Digest

- variational formulation $L = T - \Psi$
- time discretization $\mathbf{z}^k$
- discrete Lagrangian L_d
- discrete action sum S_d
- position-momentum form
  - iterative solution: $\mathbf{p}_i^k,\ \eta_j^k \quad \rightsquigarrow \quad \mathbf{r}_i^{k+1},\ \Phi_j^{k+1}$
  - update equation: $\mathbf{r}_i^{k+1},\ \Phi_j^{k+1} \quad \rightsquigarrow \quad \mathbf{p}_i^{k+1},\ \eta_j^{k+1}$

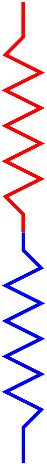
Special Cases –Thermal only

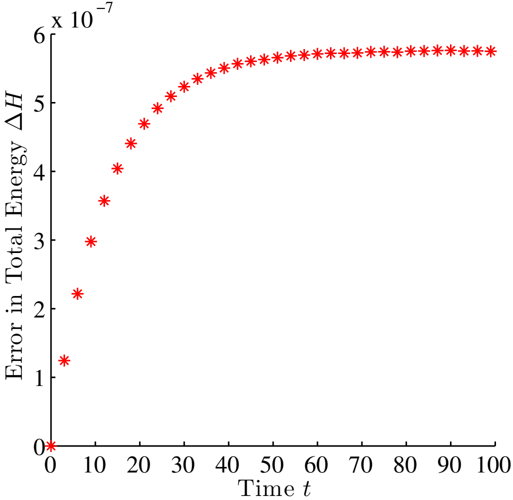




analytical and numerical (VI-GTR, $\alpha = 0.5$) solution

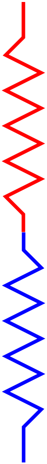
Special Cases –Thermal only

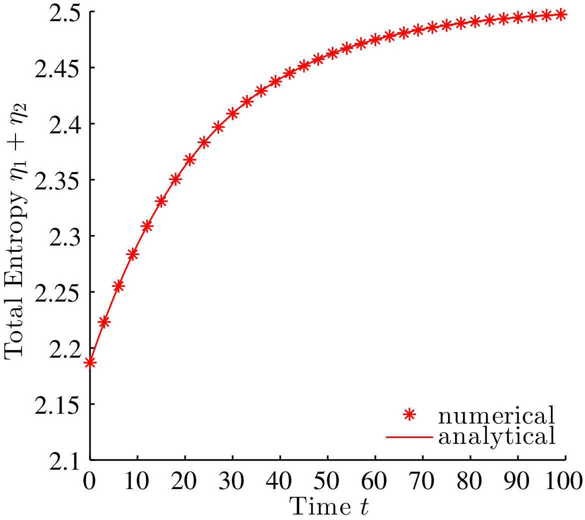




difference between numerical (VI-GTR, $\alpha = 0.5$) and analytical solution ($H = 800.015$)

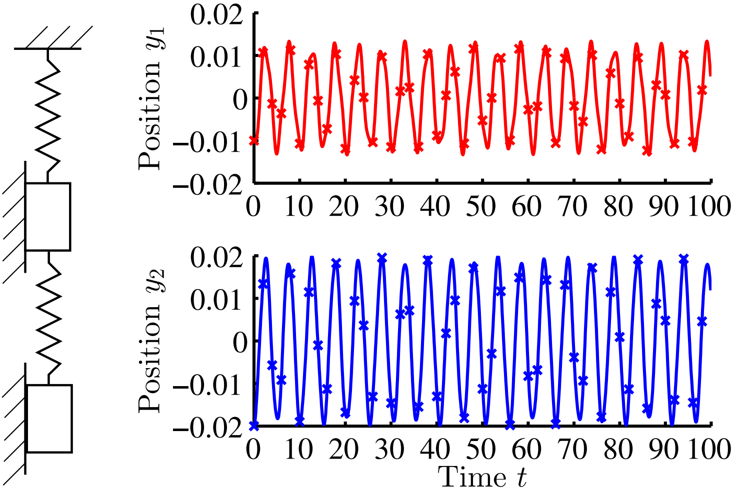
Special Cases –Thermal only





analytical and numerical (VI-GTR, $\alpha = 0.5$) solution

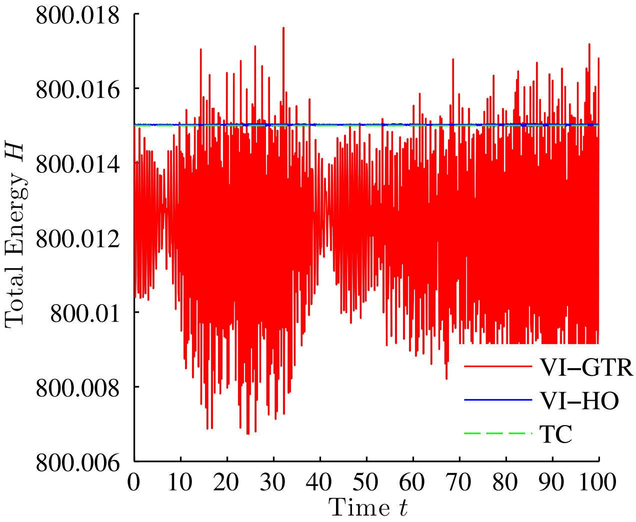
Special Cases – Mechanical only



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

Reference Results

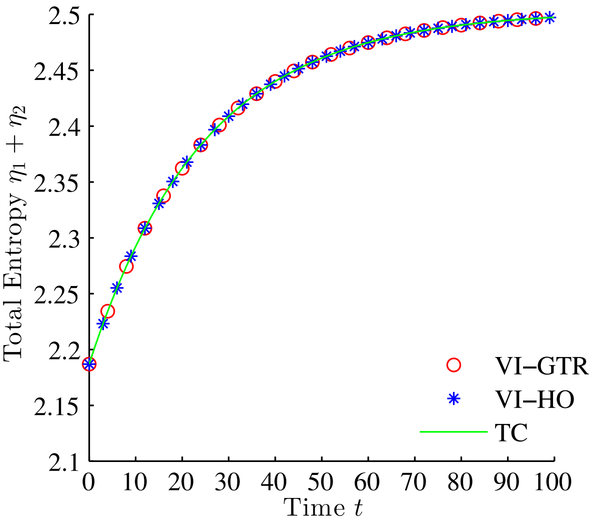
Romero [2009], Krüger & Groß & Betsch [2010], Mata & Lew [2011]



comparison between different integrators

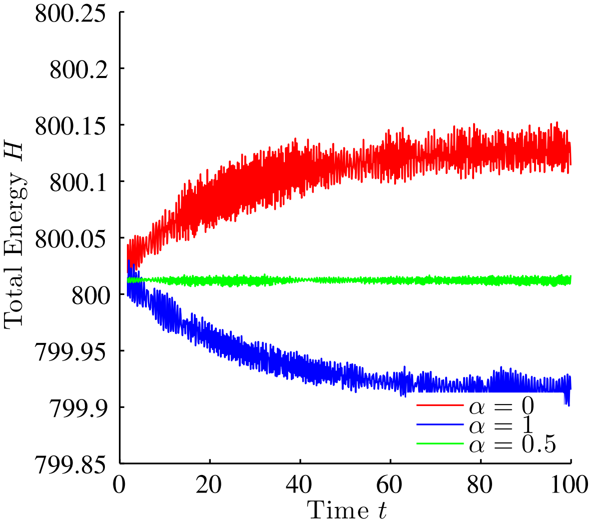
Reference Results

Romero [2009], Krüger & Groß & Betsch [2010], Mata & Lew [2011]



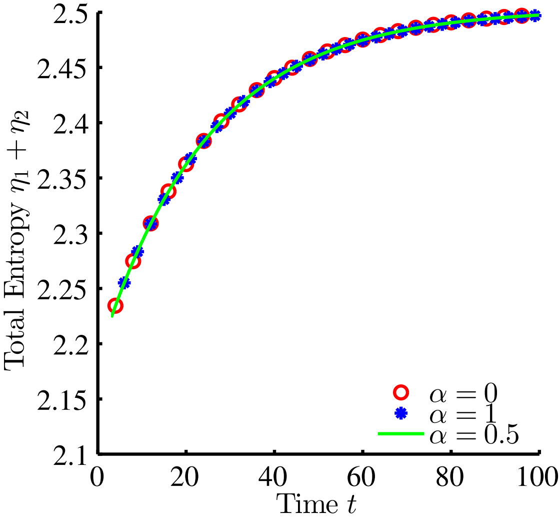
comparison between different integrators

Reference Results



comparison of different α-values of the VI-GTR integrator

Reference Results



comparison of different α-values of the VI-GTR integrator

Summary and Outlook

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).