Introduction
Outline & overview
Problem definition

Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws

Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system

Conclusions

Energy-entropy-consistent time integration of nonlinear thermo-viscoelastic continua

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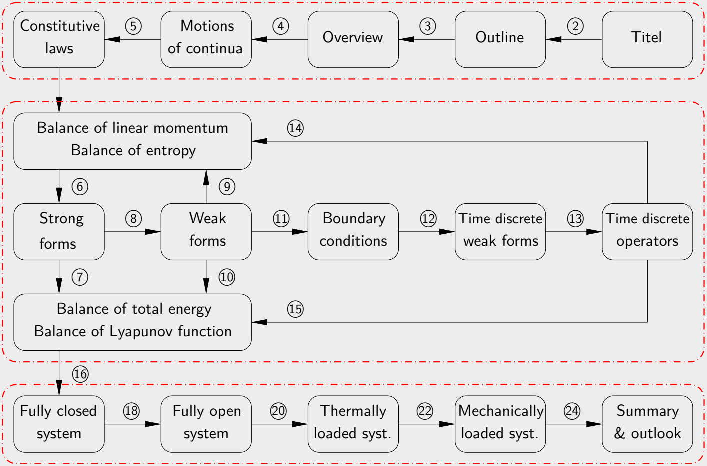
Contents of the presentation

Energy-entropy-consistent time integration of nonlinear thermo-viscoelastic continua

Melanie Krüger[1], Michael Groß & Peter Betsch[2]

Introduction
Outline & overview
Problem definition
Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws
Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system
Conclusions

Outline



▸ Goto strong forms ▸ Goto weak forms ▸ Goto balance laws ▸ Goto boundary conditions
▸ Goto time discrete weak forms ▸ Goto time discrete balance laws ▸ Goto numerical examples

Overview of structure-preserving time integrators

[1]Stuart & Humphries [1998], [2]Hairer et al. [2006], [3]Gonzalez [1996], [4]Armero & Romero [2001], [5]Marsden & West [2001], [6]Romero [2010]
[7]Betsch & Steinmann [2000], [8]Mohr et al. [2008], [9]Bauchau & Bottasso [1999], [10]Ober-Blöbaum & Saake [2013]

Characteristics

1. Preserve physical structures of (constraints on) solution spaces of time evolution equations (ODE or PDE or DAE)
2. Examples: Geometric constraints, conservation laws (e.g. energy or linear and angular momentum), balance laws (e.g. entropy, LYAPUNOV function).

Finite difference methods in time

1. Symplectic methods[1,2]
2. Energy-momentum time stepping schemes[3]
3. Energy dissipative schemes[4]
4. Variational integrators[5] (VI)
5. Energy-entropy consistent (TC) integrators[6] for thermoelastic closed systems

Finite element methods in time

1. Higher-order accurate symplectic methods[7]
2. GALERKIN-based energy-momentum methods[8]
3. GALERKIN-based energy dissipative methods[9]
4. GALERKIN-based variational integrators[10] (GVI)

Introduction
Outline & overview
Problem definition
Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws
Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system
Conclusions

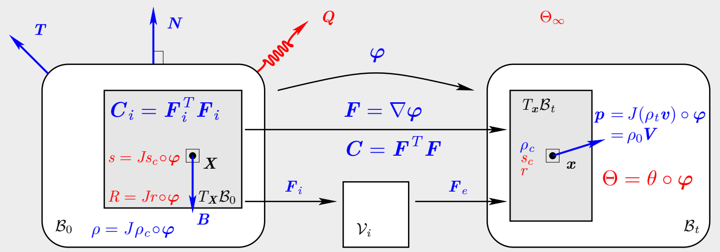
Introduction of considered continuum mechanics

Malvern [1969], Truesdell & Noll [1992], Marsden & Hughes [1994], Ogden[1997], Holzapfel [2000], Haupt [2002]

Melanie Krüger[1], Michael Groß & Peter Betsch[2]

Introduction
Outline & overview
Problem definition
Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws
Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system
Conclusions

Motion of a single isotropic continuum



State functionals

1. Total energy, total entropy & LYAPUNOV function

$$H = K + E \qquad S = \int_{\mathcal{B}_0} s \,\mathrm{d}V \qquad V = H - \Theta_\infty S$$

2. Kinetic energy & internal energy

$$K = \int_{\mathcal{B}_0} k(\boldsymbol{p}) \,\mathrm{d}V = \int_{\mathcal{B}_0} \frac{1}{2\rho} \boldsymbol{p} \cdot \boldsymbol{p} \,\mathrm{d}V \qquad E = \int_{\mathcal{B}_0} e(\boldsymbol{C}, s, \boldsymbol{C}_i) \,\mathrm{d}V$$

Constitutive laws of the considered continuum

Lu & Pister [1975], Miehe [1988], Lion [1997], Yu et al. [1997], Reese [2000], Holzapfel [2000], Vujosevic & Lubarda [2002], Heimes [2005], Hartmann [2012]

Material motion and heat conduction

1. First PIOLA-KIRCHHOFF stress tensor

$$\boldsymbol{P} = 2\,\boldsymbol{F}\,\frac{\delta E}{\delta \boldsymbol{C}} \qquad e = e^{\text{ela}}(\boldsymbol{C}) + e^{\text{the}}(\boldsymbol{C}, s) + e^{\text{vis}}(\boldsymbol{C}, \boldsymbol{C}_i)$$

2. FOURIER's law of isotropic heat conduction

$$\boldsymbol{Q} = -\kappa\, J\, \boldsymbol{C}^{-1} \nabla\Theta$$

Dissipative behaviour

1. Total dissipation

$$D^{\text{tot}} = D^{\text{cdu}} + D^{\text{vis}} = \underbrace{-\frac{1}{\Theta}\,\boldsymbol{Q}\cdot\nabla\Theta}_{\geq 0}\ \underbrace{-\frac{\delta E}{\delta \boldsymbol{C}_i} : \frac{\partial \boldsymbol{C}_i}{\partial t}}_{\geq 0} \geq 0$$

2. Viscous evolution equation

$$\boxed{\frac{\partial \boldsymbol{C}_i}{\partial t} = -\bar{\mathbb{V}}^{-1}(\boldsymbol{C}_i) : \frac{\delta E}{\delta \boldsymbol{C}_i}} \qquad \bar{\mathbb{V}}^{-1}(\boldsymbol{C}_i) = \boldsymbol{C}_i\,\mathbb{V}^{-1}\,\boldsymbol{C}_i$$

$$\mathbb{V}^{-1} = \frac{1}{2\,V^{\text{dev}}}\,\mathbb{I}^{\text{dev}^T} + \frac{1}{n_{\text{dim}}\,V^{\text{vol}}}\,\mathbb{I}^{\text{vol}}$$

Goto outline

Energy-entropy-consistent time integration of nonlinear thermo-viscoelastic continua
Melanie Krüger[1], Michael Groß & Peter Betsch[2]
Introduction
Outline & overview
Problem definition
Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws
Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system
Conclusions

Strong forms derived from the balance laws

Holzapfel [2000], Marsden & Ratiu [2000], Wriggers [2001], Maugin & Kalpakides [2002], Bargmann [2008], Mata & Lew [2011]

Equations of motion

1. Balance of total linear momentum

$$\int_{\mathcal{B}_0} \frac{\partial \boldsymbol{p}}{\partial t}\,\mathrm{d}V = \int_{\mathcal{B}_0} \boldsymbol{B}\,\mathrm{d}V + \int_{\partial\mathcal{B}_0} \boldsymbol{T}\,\mathrm{d}A \qquad \text{with} \quad \boldsymbol{T} = \boldsymbol{P}\boldsymbol{N}$$

2. Equations of motion

$$\frac{\partial \boldsymbol{p}}{\partial t} = \mathrm{Div}\,\boldsymbol{P} + \boldsymbol{B}$$

$$\frac{\partial \boldsymbol{\varphi}}{\partial t} = \frac{1}{\rho}\,\boldsymbol{p} \equiv \frac{\delta H}{\delta \boldsymbol{p}}$$

Heat conduction equations

1. Balance of total entropy

$$\int_{\mathcal{B}_0} \frac{D^{\mathrm{tot}}}{\Theta}\,\mathrm{d}V = \int_{\mathcal{B}_0} \left[\frac{\partial s}{\partial t} - \frac{R}{\Theta}\right] \mathrm{d}V + \int_{\partial\mathcal{B}_0} \frac{1}{\Theta}\,\boldsymbol{Q}\cdot\boldsymbol{N}\,\mathrm{d}A \geq 0$$

2. Heat conduction equations

$$\frac{\partial s}{\partial t} = \frac{1}{\Theta}\left[D^{\mathrm{vis}} + R - \mathrm{Div}\,\boldsymbol{Q}\right]$$

$$\Theta = \frac{\partial e}{\partial s} \equiv \frac{\delta H}{\delta s}$$

Energy-entropy-consistent time integration of nonlinear thermo-viscoelastic continua

Melanie Krüger[1], Michael Groß & Peter Betsch[2]

Introduction
Outline & overview
Problem definition
Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws
Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system
Conclusions

Introduction
Outline & overview
Problem definition
Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws
Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system
Conclusions

Strong forms and the energy balances

Truesdell & Toupin [1960], Gurtin [1975], Kestin [1979], Silhavy [1997], Wilmanski [1998]

Balance of total energy $\partial H/\partial t = P^{\mathrm{mec}} + P^{\mathrm{the}}$

1. Balance of mechanical energy

$$\int_{\mathcal{B}_0} \Big[\underbrace{\frac{\delta H}{\delta \boldsymbol{p}} \cdot \frac{\partial \boldsymbol{p}}{\partial t}}_{\partial k/\partial t} + \underbrace{\frac{\delta H}{\delta \boldsymbol{F}} : \frac{\partial \boldsymbol{F}}{\partial t}}_{p^{\mathrm{int}}} \Big] \mathrm{d}V \underbrace{=}_{\text{eqns. of motion}} \underbrace{\int_{\mathcal{B}_0} \frac{\partial \boldsymbol{\varphi}}{\partial t} \cdot \boldsymbol{B}\, \mathrm{d}V + \int_{\partial \mathcal{B}_0} \frac{\partial \boldsymbol{\varphi}}{\partial t} \cdot \boldsymbol{T}\, \mathrm{d}A}_{P^{\mathrm{mec}}}$$

2. Balance of thermal energy

$$\int_{\mathcal{B}_0} \Big[\underbrace{\frac{\delta H}{\delta s} \frac{\partial s}{\partial t}}_{p^{\mathrm{ent}}} + \underbrace{\frac{\delta H}{\delta \boldsymbol{C}_i} : \frac{\partial \boldsymbol{C}_i}{\partial t}}_{-D^{\mathrm{vis}}} \Big] \mathrm{d}V \underbrace{=}_{\text{heat cond. eqns.}} \underbrace{\int_{\mathcal{B}_0} R\, \mathrm{d}V - \int_{\partial \mathcal{B}_0} \boldsymbol{Q} \cdot \boldsymbol{N}\, \mathrm{d}A}_{P^{\mathrm{the}}}$$

Balance of LYAPUNOV function $V = H - \Theta_\infty S$

$$\frac{\partial V}{\partial t} \equiv \underbrace{\frac{\partial H}{\partial t}}_{\text{total energy balance}} - \Theta_\infty \int_{\mathcal{B}_0} \underbrace{\frac{\partial s}{\partial t}}_{\text{heat cond. eqn.}} \mathrm{d}V$$

$$\frac{\partial V}{\partial t} = -\int_{\mathcal{B}_0} \frac{\Theta_\infty}{\Theta} D^{\mathrm{tot}}\, \mathrm{d}V + \int_{\mathcal{B}_0} \frac{\partial \boldsymbol{\varphi}}{\partial t} \cdot \boldsymbol{B}\, \mathrm{d}V + \int_{\partial \mathcal{B}_0} \frac{\partial \boldsymbol{\varphi}}{\partial t} \cdot \boldsymbol{T}\, \mathrm{d}A$$
$$+ \int_{\mathcal{B}_0} \frac{\Theta - \Theta_\infty}{\Theta} R\, \mathrm{d}V - \int_{\partial \mathcal{B}_0} \frac{\Theta - \Theta_\infty}{\Theta} \boldsymbol{Q} \cdot \boldsymbol{N}\, \mathrm{d}A \qquad (\leq 0)$$

Goto outline

Weak forms derived from the strong forms

Willner [1990], Miehe [1993], Gonzalez [1996], Simo [1998], Reese [2000], Romero [2010a,2010b], Krüger [2012]

Introduction
Outline & overview
Problem definition
Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws
Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system
Conclusions

Weak equations of motion (integration by parts)

$$\int_{\mathcal{B}_0}\left[\delta\boldsymbol{\varphi}\cdot\frac{\partial\boldsymbol{p}}{\partial t}+\nabla(\delta\boldsymbol{\varphi}):\frac{\delta H}{\delta\boldsymbol{F}}\right]\mathrm{d}V=\int_{\mathcal{B}_0}\delta\boldsymbol{\varphi}\cdot\boldsymbol{B}\,\mathrm{d}V+\int_{\partial\mathcal{B}_0}\delta\boldsymbol{\varphi}\cdot\boldsymbol{T}\,\mathrm{d}A$$

$$\int_{\mathcal{B}_0}\delta\boldsymbol{p}\cdot\left[\frac{\partial\boldsymbol{\varphi}}{\partial t}-\frac{\delta H}{\delta\boldsymbol{p}}\right]\mathrm{d}V=0$$

Weak heat conduction equations

$$-\int_{\mathcal{B}_0}\frac{\delta\Theta}{\Theta}\,\mathrm{Div}\,\boldsymbol{Q}\,\mathrm{d}V\underbrace{=}_{\substack{\text{integration by parts}\\ \text{GAUSS theorem}}}\int_{\mathcal{B}_0}\nabla\left(\frac{\delta\Theta}{\Theta}\right)\cdot\boldsymbol{Q}\,\mathrm{d}V-\int_{\partial\mathcal{B}_0}\frac{\delta\Theta}{\Theta}\,\boldsymbol{Q}\cdot\boldsymbol{N}\,\mathrm{d}A$$

$$\int_{\mathcal{B}_0}\left[\delta\Theta\,\frac{\partial s}{\partial t}+\frac{\delta\Theta}{\Theta}\underbrace{\frac{\delta H}{\delta\boldsymbol{C}_i}:\frac{\partial\boldsymbol{C}_i}{\partial t}}_{-D^{\mathrm{vis}}}\right]\mathrm{d}V=\int_{\mathcal{B}_0}\left[\frac{\delta\Theta}{\Theta}R+\nabla\left(\frac{\delta\Theta}{\Theta}\right)\cdot\boldsymbol{Q}\right]\mathrm{d}V-\int_{\partial\mathcal{B}_0}\frac{\delta\Theta}{\Theta}\,\boldsymbol{Q}\cdot\boldsymbol{N}\,\mathrm{d}A$$

$$\int_{\mathcal{B}_0}\delta s\left[\Theta-\frac{\delta H}{\delta s}\right]\mathrm{d}V=0$$

Goto outline

Weak forms fulfill all balance laws (I)

Melanie Krüger[1], Michael Groß & Peter Betsch[2]

Introduction
Outline & overview
Problem definition
Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws
Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system
Conclusions

Balance of total linear momentum

Choose $\delta\boldsymbol{\varphi}(\boldsymbol{X},t) = \boldsymbol{c} = \text{const.}$

$$\underbrace{\boldsymbol{c}\cdot\left[\int_{\mathcal{B}_0}\left[\frac{\partial \boldsymbol{p}}{\partial t} - \boldsymbol{B}\right]\mathrm{d}V - \int_{\partial\mathcal{B}_0}\boldsymbol{T}\,\mathrm{d}A\right]}_{\text{Balance of linear momentum}} = 0$$

Balance of total entropy

Choose $\delta\Theta(\boldsymbol{X},t) = \Theta_\infty = \text{const.}$

$$\underbrace{\Theta_\infty\left[\int_{\mathcal{B}_0}\left[\frac{\partial s}{\partial t} - \frac{D^{\text{vis}} + R}{\Theta} - \overbrace{\nabla\left(\frac{1}{\Theta}\right)\cdot\boldsymbol{Q}}^{D^{\text{cdu}}/\Theta}\right]\mathrm{d}V + \int_{\partial\mathcal{B}_0}\frac{1}{\Theta}\boldsymbol{Q}\cdot\boldsymbol{N}\,\mathrm{d}A\right]}_{\text{Entropy inequality principle with } D^{\text{tot}} \geq 0} = 0$$

Balance of mechanical energy

Choose $\delta\boldsymbol{\varphi}(\boldsymbol{X},t) = \frac{\partial\boldsymbol{\varphi}(\boldsymbol{X},t)}{\partial t}$ and $\delta\boldsymbol{p}(\boldsymbol{X},t) = \frac{\partial\boldsymbol{p}(\boldsymbol{X},t)}{\partial t}$

$$\underbrace{\int_{\mathcal{B}_0}\left[\overbrace{\frac{\delta H}{\delta \boldsymbol{p}}\cdot\frac{\partial \boldsymbol{p}}{\partial t}}^{\partial k/\partial t} + \overbrace{\frac{\delta H}{\delta \boldsymbol{F}} : \frac{\partial \boldsymbol{F}}{\partial t}}^{p^{\text{int}}}\right]\mathrm{d}V = \overbrace{\int_{\mathcal{B}_0}\frac{\partial\boldsymbol{\varphi}}{\partial t}\cdot\boldsymbol{B}\,\mathrm{d}V + \int_{\partial\mathcal{B}_0}\frac{\partial\boldsymbol{\varphi}}{\partial t}\cdot\boldsymbol{T}\,\mathrm{d}A}^{P^{\text{mec}}}}_{\text{Balance of mechanical energy}}$$

Weak forms fulfill all balance laws (II)

Balance of thermal energy

Choose $\delta\Theta(\boldsymbol{X},t) = \Theta(\boldsymbol{X},t)$ and $\delta s(\boldsymbol{X},t) = \frac{\partial s(\boldsymbol{X},t)}{\partial t}$

$$\underbrace{\int_{\mathcal{B}_0} \Bigg[\overbrace{\frac{\delta H}{\delta s}\,\frac{\partial s}{\partial t}}^{p^{\text{ent}}} + \overbrace{\frac{\delta H}{\delta \boldsymbol{C}_i} : \frac{\partial \boldsymbol{C}_i}{\partial t}}^{-D^{\text{vis}}} \Bigg] \mathrm{d}V = \overbrace{\int_{\mathcal{B}_0} R \,\mathrm{d}V - \int_{\partial\mathcal{B}_0} \boldsymbol{Q}\cdot\boldsymbol{N}\,\mathrm{d}A}^{P^{\text{the}}}}_{\text{Balance of thermal energy}}$$

Balance of total energy

Add balance of mechanical and thermal energy

$$\underbrace{\frac{\partial H}{\partial t} = \int_{\mathcal{B}_0} \left[\frac{\partial \varphi}{\partial t} \cdot \boldsymbol{B} + R \right] \mathrm{d}V + \int_{\partial\mathcal{B}_0} \left[\frac{\partial \varphi}{\partial t} \cdot \boldsymbol{T} - \boldsymbol{Q}\cdot\boldsymbol{N} \right] \mathrm{d}A}_{\text{Balance of total energy}}$$

Balance of Lyapunov function

1. Choose $\delta\Theta(\boldsymbol{X},t) = \Theta(\boldsymbol{X},t) - \Theta_\infty$, $\delta s(\boldsymbol{X},t) = \frac{\partial s(\boldsymbol{X},t)}{\partial t}$ and add the balance of mechanical energy (without entropy and total energy consistency possible, cp. ehG method).

or 2.
$$\frac{\partial V}{\partial t} = \underbrace{\frac{\partial H}{\partial t}}_{\text{Balance of total energy}} \underbrace{- \Theta_\infty \int_{\mathcal{B}_0} \frac{\partial s}{\partial t}\,\mathrm{d}V}_{\text{Balance of total entropy}}$$

Goto outline

Energy-entropy-consistent time integration of nonlinear thermo-viscoelastic continua

Melanie Krüger[1], Michael Groß & Peter Betsch[2]

Introduction
Outline & overview
Problem definition
Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws
Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system
Conclusions

Energy-entropy-consistent time integration of nonlinear thermo-viscoelastic continua

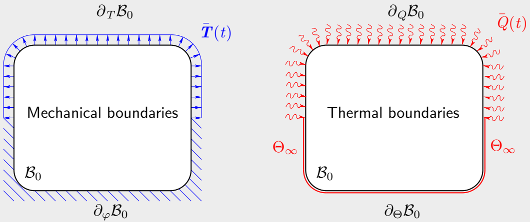
Melanie Krüger[1], Michael Groß & Peter Betsch[2]

Introduction
Outline & overview
Problem definition
Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws
Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system
Conclusions

Boundary conditions in the weak forms

Babuska [1973], Kikuchi & Oden [1988], Farhat & Geradin [1992], Glowinski et al. [1994], Stenberg [1995], Wriggers [2002], Donea & Huerta [2003], Hartmann et al. [2008]

Boundary conditions



Mechanical boundary

$$\int_{\partial\mathcal{B}_0} \delta\boldsymbol{\varphi}\cdot\boldsymbol{T}\,\mathrm{d}A = \int_{\partial_\varphi\mathcal{B}_0} \underbrace{\delta\boldsymbol{\varphi}}_{=:0}\cdot\boldsymbol{T}\,\mathrm{d}A + \int_{\partial_T\mathcal{B}_0} \delta\boldsymbol{\varphi}\cdot\bar{\boldsymbol{T}}(t)\,\mathrm{d}A$$

Thermal boundary (with LAGRANGE multiplier technique)

$$\int_{\partial\mathcal{B}_0} \frac{\delta\Theta}{\Theta}\boldsymbol{Q}\cdot\boldsymbol{N}\,\mathrm{d}A = \int_{\partial_\Theta\mathcal{B}_0} \delta\Theta\,\lambda_\Theta\,\mathrm{d}A - \int_{\partial_Q\mathcal{B}_0} \frac{\delta\Theta}{\Theta}\bar{Q}(t)\,\mathrm{d}A$$

with

$$\int_{\partial_\Theta\mathcal{B}_0} \delta\lambda_\Theta\,[\Theta-\Theta_\infty]\,\mathrm{d}A = 0 \qquad \lambda_\Theta : \text{LAGRANGE multiplier (outward normal entropy flux)}$$

Goto outline

Time discrete weak forms (2^{nd} order accurate)

Simo & Tarnow [1992], Simo & Hughes [1998], Betsch & Steinmann [2002], Ibrahimbegovic & Mamouri [2002], Armero [2006], Romero [2010], Hesch & Betsch [2011]

Equations of motion

$$\int_{\mathcal{B}_0} \delta \boldsymbol{p}_{n+1} \cdot \left[\frac{\Delta \boldsymbol{\varphi}}{\Delta t} - \frac{\Delta^P H}{\Delta \boldsymbol{p}} \right] \mathrm{d}V = 0$$

$$\int_{\mathcal{B}_0} \left[\delta \boldsymbol{\varphi}_{n+1} \cdot \frac{\Delta \boldsymbol{p}}{\Delta t} + \nabla(\delta \boldsymbol{\varphi}_{n+1}) : \frac{\Delta^P H}{\Delta \boldsymbol{F}} \right] \mathrm{d}V = \int_{\mathcal{B}_0} \delta \boldsymbol{\varphi}_{n+1} \cdot \boldsymbol{B}_{\frac{1}{2}} \, \mathrm{d}V + \int_{\partial_T \mathcal{B}_0} \delta \boldsymbol{\varphi}_{n+1} \cdot \bar{\boldsymbol{T}}_{\frac{1}{2}} \, \mathrm{d}A$$

Heat conduction equations

$$\int_{\mathcal{B}_0} \delta s_{n+1} \cdot \left[\Theta_{n+1} - \frac{\Delta^P H}{\Delta s} \right] \mathrm{d}V = 0$$

$$\int_{\mathcal{B}_0} \left[\delta \Theta_{n+1} \frac{\Delta s}{\Delta t} + \frac{\delta \Theta_{n+1}}{\Theta_{n+1}} \frac{\Delta^P H}{\Delta \boldsymbol{C}_i} : \frac{\Delta \boldsymbol{C}_i}{\Delta t} \right] \mathrm{d}V = \int_{\mathcal{B}_0} \left[\nabla \left(\frac{\delta \Theta_{n+1}}{\Theta_{n+1}} \right) \cdot \boldsymbol{Q}_{\frac{1}{2}} + \frac{\delta \Theta_{n+1}}{\Theta_{n+1}} R_{\frac{1}{2}} \right] \mathrm{d}V + \int_{\partial_\Theta \mathcal{B}_0} \delta \Theta_{n+1} \, \lambda_{n+1} \, \mathrm{d}A + \int_{\partial_Q \mathcal{B}_0} \frac{\delta \Theta_{n+1}}{\Theta_{n+1}} \bar{Q}_{\frac{1}{2}} \, \mathrm{d}A$$

Local and boundary time evolutions

1. Viscous evolution $\quad \dfrac{\Delta \boldsymbol{C}_i}{\Delta t} + \bar{\mathbb{V}}^{-1}(\boldsymbol{C}_{i_{n+\frac{1}{2}}}) : \dfrac{\Delta^P H}{\Delta \boldsymbol{C}_i} = 0$
2. Boundary condition $\quad \displaystyle\int_{\partial_\Theta \mathcal{B}_0} \delta \lambda_{n+1} \left[\Theta_{n+1} - \Theta_\infty \right] \mathrm{d}A = 0$

Energy-entropy-consistent time integration of nonlinear thermo-viscoelastic continua

Melanie Krüger[1], Michael Groß & Peter Betsch[2]

Introduction
Outline & overview
Problem definition
Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws
Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system
Conclusions

Time discrete operators (2^{nd} order accurate)

Milne-Thomson [1933], Greenspan [1973], LaBudde & Greenspan [1974], Simo & Gonzalez [1993], Gonzalez [1996a, 1996b], Sansour et al. [2004], Bourdin & Cresson [2012]

Introduction
Outline & overview
Problem definition
Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws
Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system
Conclusions

Single-variable function discrete derivative of $\boldsymbol{f}(\boldsymbol{z})$

$$\boldsymbol{f} \in \{k, s, \boldsymbol{p}, \boldsymbol{\varphi}, \boldsymbol{C}_i\} \qquad \boldsymbol{z} \in \{t, s, \boldsymbol{p}, \boldsymbol{C}, \boldsymbol{C}_i\} \qquad \odot \in \{\ , \cdot, :\}$$

$$\frac{\Delta \boldsymbol{f}}{\Delta \boldsymbol{z}} = \frac{\partial \boldsymbol{f}(\boldsymbol{z}_{n+\frac{1}{2}})}{\partial \boldsymbol{z}} + \frac{\boldsymbol{f}(\boldsymbol{z}_{n+1}) - \boldsymbol{f}(\boldsymbol{z}_n) - \dfrac{\partial \boldsymbol{f}(\boldsymbol{z}_{n+\frac{1}{2}})}{\partial \boldsymbol{z}} \odot [\boldsymbol{z}_{n+1} - \boldsymbol{z}_n]}{[\boldsymbol{z}_{n+1} - \boldsymbol{z}_n] \odot [\boldsymbol{z}_{n+1} - \boldsymbol{z}_n]} [\boldsymbol{z}_{n+1} - \boldsymbol{z}_n]$$

Special case 1: Scalar-valued $\boldsymbol{z}$: $\quad \dfrac{\Delta \boldsymbol{f}}{\Delta t} = \dfrac{\boldsymbol{f}(\boldsymbol{z}_{n+1}) - \boldsymbol{f}(\boldsymbol{z}_n)}{t_{n+1} - t_n}$

Special case 2: Quadratic $\boldsymbol{f}$: $\quad \dfrac{\Delta k}{\Delta \boldsymbol{p}} = \dfrac{\partial k(\boldsymbol{p}_{n+\frac{1}{2}})}{\partial \boldsymbol{p}} \equiv \dfrac{1}{\rho} \boldsymbol{p}_{n+\frac{1}{2}}$

Multi-variable functional (partitioned) discrete derivatives

$$\frac{\Delta^P H}{\Delta \boldsymbol{p}} = \frac{\Delta k}{\Delta \boldsymbol{p}} \quad \text{with} \quad k(\boldsymbol{p}) \quad \text{and} \quad e(\boldsymbol{C}, s, \boldsymbol{C}_i)$$

$$\frac{\Delta^P H}{\Delta \boldsymbol{F}} = \boldsymbol{F}_{n+\frac{1}{2}} \left[\frac{\Delta e}{\Delta \boldsymbol{C}}\bigg|_{s_n, \boldsymbol{C}_{i_n}} + \frac{\Delta e}{\Delta \boldsymbol{C}}\bigg|_{s_{n+1}, \boldsymbol{C}_{i_{n+1}}} \right]$$

$$\frac{\Delta^P H}{\Delta s} = \frac{1}{2} \left[\frac{\Delta e}{\Delta s}\bigg|_{\boldsymbol{C}_n, \boldsymbol{C}_{i_{n+1}}} + \frac{\Delta e}{\Delta s}\bigg|_{\boldsymbol{C}_{n+1}, \boldsymbol{C}_{i_n}} \right]$$

$$\frac{\Delta^P H}{\Delta \boldsymbol{C}_i} = \frac{1}{2} \left[\frac{\Delta e}{\Delta \boldsymbol{C}_i}\bigg|_{\boldsymbol{C}_n, s_n} + \frac{\Delta e}{\Delta \boldsymbol{C}_i}\bigg|_{\boldsymbol{C}_{n+1}, s_{n+1}} \right]$$

Goto outline

Time discrete balance laws (I)

Balance of total linear momentum

Choose $\delta\boldsymbol{\varphi}_{n+1}(\boldsymbol{X}) = \boldsymbol{c} = \text{const.}$

$$\boldsymbol{c}\cdot\underbrace{\left[\int_{\mathcal{B}_0}\left[\frac{\Delta\boldsymbol{p}}{\Delta t}-\boldsymbol{B}_{\frac{1}{2}}\right]\mathrm{d}V-\int_{\partial_T\mathcal{B}_0}\bar{\boldsymbol{T}}_{\frac{1}{2}}\,\mathrm{d}A\right]}_{\text{Time discrete balance of linear momentum}}=0$$

Balance of total entropy

Choose $\delta\Theta_{n+1}(\boldsymbol{X}) = \Theta_\infty = \text{const.}$

$$\Theta_\infty\underbrace{\left[\int_{\mathcal{B}_0}\left[\frac{\Delta s}{\Delta t}-\frac{D^{\text{tot}}_{\frac{1}{2}}+R_{\frac{1}{2}}}{\Theta_{n+1}}\right]\mathrm{d}V+\int_{\partial_\Theta\mathcal{B}_0}\lambda_{n+1}\,\mathrm{d}A-\int_{\partial_Q\mathcal{B}_0}\frac{\bar{Q}_{\frac{1}{2}}}{\Theta_{n+1}}\,\mathrm{d}A\right]}_{\text{Time discrete entropy inequality principle with } D^{\text{tot}}_{\frac{1}{2}}\geq 0}=0$$

Balance of mechanical energy

Choose $\delta\boldsymbol{\varphi}_{n+1}(\boldsymbol{X}) = \frac{\Delta\boldsymbol{\varphi}(\boldsymbol{X})}{\Delta t}$ and $\delta\boldsymbol{p}_{n+1}(\boldsymbol{X}) = \frac{\Delta\boldsymbol{p}(\boldsymbol{X})}{\Delta t}$

$$\underbrace{\frac{\Delta K}{\Delta t}+\frac{1}{2}\left[\left.\frac{\Delta E}{\Delta t}\right|_{s_n,\boldsymbol{C}_{i_n}}+\left.\frac{\Delta E}{\Delta t}\right|_{s_{n+1},\boldsymbol{C}_{i_{n+1}}}\right]=\int_{\mathcal{B}_0}\frac{\Delta\boldsymbol{\varphi}}{\Delta t}\cdot\boldsymbol{B}_{\frac{1}{2}}\,\mathrm{d}V+\int_{\partial_T\mathcal{B}_0}\frac{\Delta\boldsymbol{\varphi}}{\Delta t}\cdot\bar{\boldsymbol{T}}_{\frac{1}{2}}\,\mathrm{d}A}_{\text{Time discrete balance of mechanical energy}}$$

Energy-entropy-consistent time integration of nonlinear thermo-viscoelastic continua

Melanie Krüger[1], Michael Groß & Peter Betsch[2]

Introduction
Outline & overview
Problem definition
Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws
Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system
Conclusions

Time discrete balance laws (II)

Balance of thermal energy

Choose $\delta\Theta_{n+1}(\boldsymbol{X}) = \Theta_{n+1}(\boldsymbol{X})$, $\delta s_{n+1}(\boldsymbol{X}) = \frac{\Delta s(\boldsymbol{X})}{\Delta t}$ and $\delta\lambda_{n+1}(\boldsymbol{X}) = \lambda_{n+1}(\boldsymbol{X})$

$$\underbrace{\frac{1}{2}\left[\left.\frac{\Delta E}{\Delta t}\right|_{\boldsymbol{C}_n,\boldsymbol{C}_{i_{n+1}}} + \left.\frac{\Delta E}{\Delta t}\right|_{\boldsymbol{C}_{n+1},\boldsymbol{C}_{i_n}} + \left.\frac{\Delta E}{\Delta t}\right|_{\boldsymbol{C}_n,s_n} + \left.\frac{\Delta E}{\Delta t}\right|_{\boldsymbol{C}_{n+1},s_{n+1}}\right] = \int_{\mathcal{B}_0} R_{\frac{1}{2}}\,\mathrm{d}V - \Theta_\infty \int_{\partial_\Theta\mathcal{B}_0} \lambda_{n+1}\,\mathrm{d}A + \int_{\partial_Q\mathcal{B}_0} \bar{Q}_{\frac{1}{2}}\,\mathrm{d}A}_{\text{Time discrete balance of thermal energy}}$$

Balance of total energy

Add time discrete balance of mechanical and thermal energy

$$\underbrace{\frac{\Delta H}{\Delta t} = \int_{\mathcal{B}_0}\left[\frac{\Delta\boldsymbol{\varphi}}{\Delta t}\cdot\boldsymbol{B}_{\frac{1}{2}} + R_{\frac{1}{2}}\right]\mathrm{d}V + \int_{\partial_T\mathcal{B}_0}\frac{\Delta\boldsymbol{\varphi}}{\Delta t}\cdot\bar{\boldsymbol{T}}_{\frac{1}{2}}\,\mathrm{d}A - \Theta_\infty\int_{\partial_\Theta\mathcal{B}_0}\lambda_{n+1}\,\mathrm{d}A + \int_{\partial_Q\mathcal{B}_0}\bar{Q}_{\frac{1}{2}}\,\mathrm{d}A}_{\text{Time discrete balance of total energy}}$$

Balance of Lyapunov function (Lagrange multiplier will be eliminated)

1. Choose $\delta\Theta_{n+1}(\boldsymbol{X}) = \Theta_{n+1}(\boldsymbol{X}) - \Theta_\infty$, $\delta s_{n+1}(\boldsymbol{X}) = \frac{\Delta s(\boldsymbol{X})}{\Delta t}$, $\delta\lambda_{n+1}(\boldsymbol{X}) = \lambda_{n+1}(\boldsymbol{X})$ and add the time discrete balance of mechanical energy (cp. ehG method)

or 2. $$\frac{\Delta V}{\Delta t} = \underbrace{\frac{\Delta H}{\Delta t}}_{\text{Time discrete balance of total energy}} - \underbrace{\Theta_\infty\int_{\mathcal{B}_0}\frac{\Delta s}{\Delta t}\,\mathrm{d}V}_{\text{Time discrete balance of total entropy}}$$

Goto outline

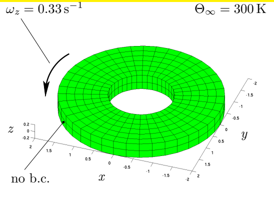
Energy-entropy-consistent time integration of nonlinear thermo-viscoelastic continua
Melanie Krüger[1], Michael Groß & Peter Betsch[2]
Introduction
Outline & overview
Problem definition
Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws
Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system
Conclusions

Free rotating insulated thermo-viscoelastic disc

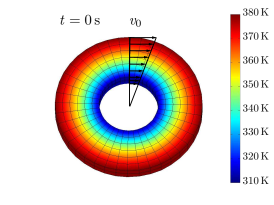
Melanie Krüger[1], Michael Groß & Peter Betsch[2]

Introduction
Outline & overview
Problem definition
Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws
Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system
Conclusions

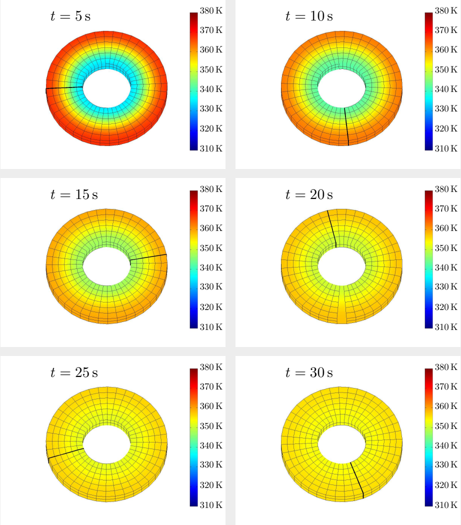
Boundary conditions



Reference configuration



ETC integrator with $\Delta t = 0.02\,\mathrm{s}$



Free rotating insulated thermo-viscoelastic disc

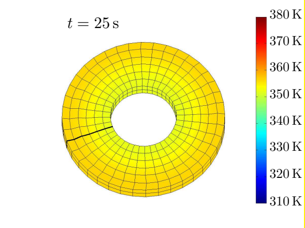
Introduction
- Outline & overview
- Problem definition

Theoretical studies
- Strong forms & balances
- Weak forms & balance laws
- Boundary conditions
- Time discrete weak forms
- Time discrete operators
- Time discrete balance laws

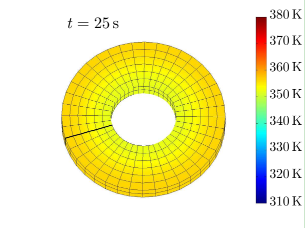
Numerical studies
- **Fully closed system**
- Fully open system
- Thermally loaded system
- Mechanically loaded system

Conclusions

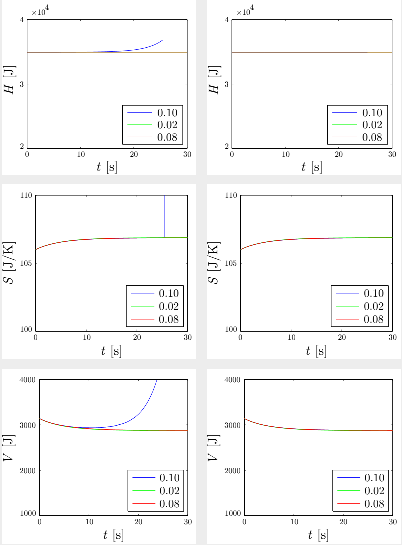
Midpoint rule ($\Delta t = 0.1\,\mathrm{s}$)



ETC integrator ($\Delta t = 0.1\,\mathrm{s}$)



Midpoint rule | ETC integrator

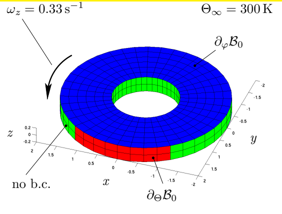


Rail-bound uninsulated thermo-viscoelastic disc

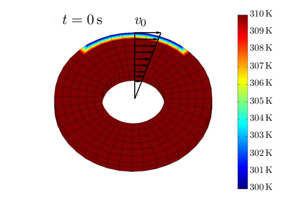
Melanie Krüger[1], Michael Groß & Peter Betsch[2]

Introduction
Outline & overview
Problem definition
Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws
Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system
Conclusions

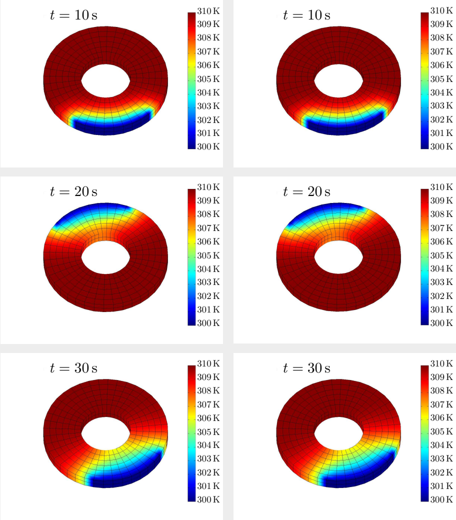
Boundary conditions



Reference configuration



MPR $(\Delta t = 0.02\,\mathrm{s})$ ETC $(\Delta t = 0.02\,\mathrm{s})$

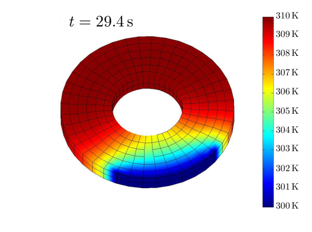


Rail-bound uninsulated thermo-viscoelastic disc

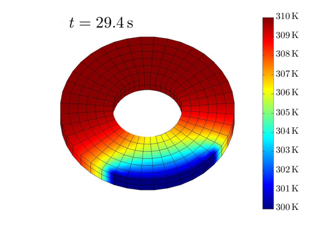
Melanie Krüger[1], Michael Groß & Peter Betsch[2]

Introduction
Outline & overview
Problem definition
Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws
Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system
Conclusions

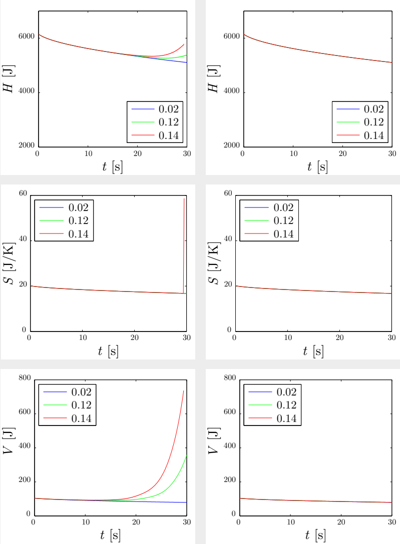
Midpoint rule ($\Delta t = 0.14\,\mathrm{s}$)



ETC integrator ($\Delta t = 0.14\,\mathrm{s}$)



Midpoint rule / ETC integrator



Thermo-viscoelastic disc with heat exchange

Energy-entropy-consistent time integration of nonlinear thermo-viscoelastic continua

Melanie Krüger[1], Michael Groß & Peter Betsch[2]

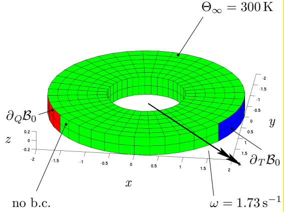
Introduction
- Outline & overview
- Problem definition

Theoretical studies
- Strong forms & balances
- Weak forms & balance laws
- Boundary conditions
- Time discrete weak forms
- Time discrete operators
- Time discrete balance laws

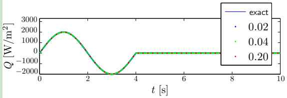
Numerical studies
- Fully closed system
- Fully open system
- Thermally loaded system
- Mechanically loaded system

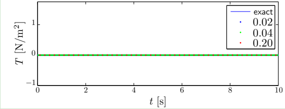
Conclusions

Boundary conditions

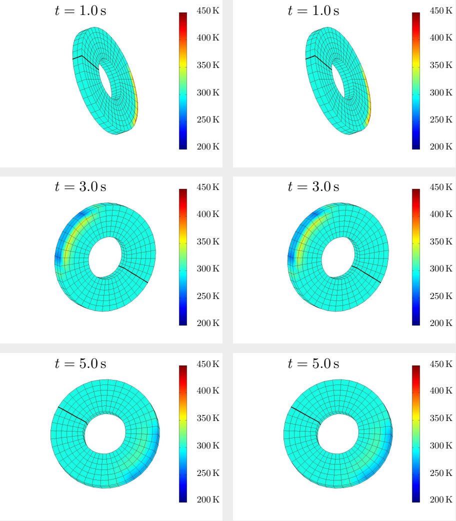


Load history





MPR ($\Delta t = 0.02\,\mathrm{s}$) ETC ($\Delta t = 0.02\,\mathrm{s}$)



Thermo-viscoelastic disc with heat exchange

Energy-entropy-consistent time integration of nonlinear thermo-viscoelastic continua

Melanie Krüger[1], Michael Groß & Peter Betsch[2]

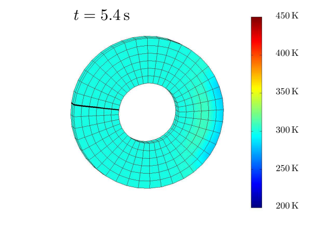
Introduction
Outline & overview
Problem definition

Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws

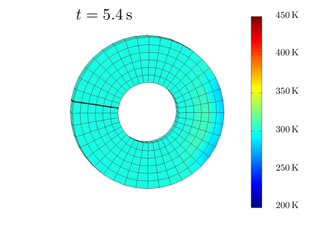
Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system

Conclusions

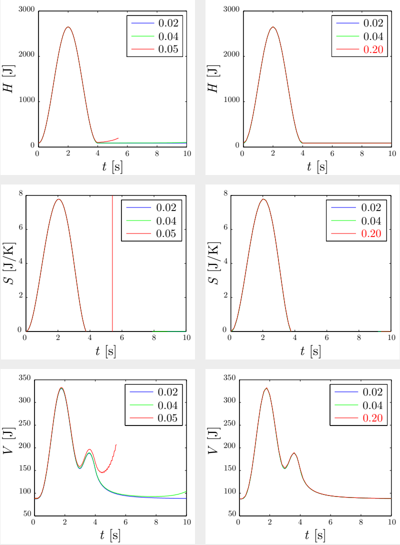
Midpoint rule ($\Delta t = 0.05\,\mathrm{s}$)



ETC integrator ($\Delta t = 0.20\,\mathrm{s}$)



Midpoint rule | ETC integrator



Thermo-viscoelastic compression buffer

Energy-entropy-consistent time integration of nonlinear thermo-viscoelastic continua

Melanie Krüger[1], Michael Groß & Peter Betsch[2]

Introduction
- Outline & overview
- Problem definition

Theoretical studies
- Strong forms & balances
- Weak forms & balance laws
- Boundary conditions
- Time discrete weak forms
- Time discrete operators
- Time discrete balance laws

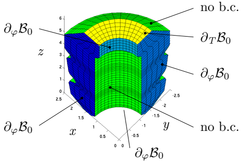
Numerical studies
- Fully closed system
- Fully open system
- Thermally loaded system
- Mechanically loaded system

Conclusions

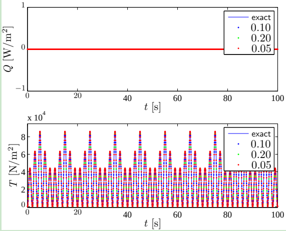
Boundary conditions

bottom supported $\quad \boldsymbol{v} = \mathbf{0}\,\mathrm{s}^{-1} \quad$ top loaded

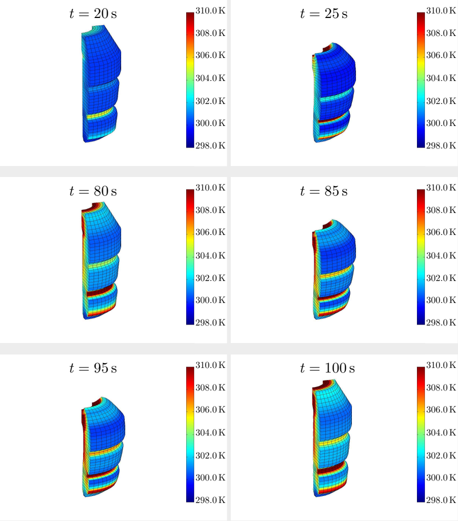
$\Theta_0 = \Theta_\infty = 300\,\mathrm{K}$



Load history



ETC ($\Delta t = 0.1\,\mathrm{s}$)

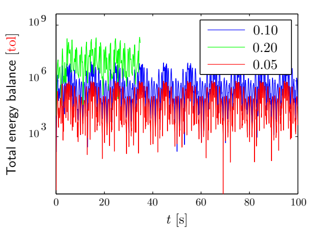


Thermo-viscoelastic compression buffer

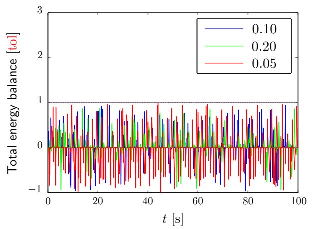
Melanie Krüger[1], Michael Groß & Peter Betsch[2]

Introduction
Outline & overview
Problem definition
Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws
Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system
Conclusions

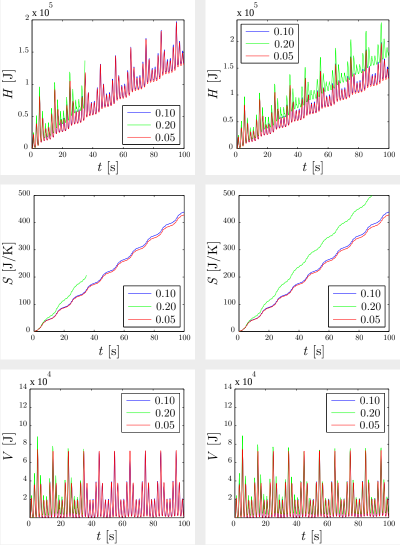
Midpoint rule



ETC integrator



Midpoint rule | ETC integrator



Conclusions

[1]Maugin & Kalpakides [2002], Bargmann [2008] [2]Zielonka [2006], Zielonka, Ortiz & Marsden [2008], Mata & Lew [2011]
[3]Ibrahimbegovic, Chorfi & Gharzeddine [2001], Hartmann, Quint & Arnold [2008], Birken et al. [2010], Moore [2011], Gleim & Kuhl [2013]

Summary

1. Goal: The ETC integrator fulfills
   - the balance of total linear/angular momentum AND total entropy
   - the balance of total energy AND LYAPUNOV function

   also with DIRICHLET and NEUMANN boundary conditions.
2. Algorithmic basis: A spatially weak formulation, which fulfills
   - ALL balance laws for STANDARD finite element spaces
3. Algorithmic key: A time discretisation with
   - time discrete differential operators which satisfy the discrete version of the fundamental theorem of calculus.
4. Benefit: A transient simulation with an improved
   - numerical stability for large time steps, and
   - physically consistent solutions (NO hour-glassing, NO waves)

Outlook

5. Introduction of a (mixed) variational formulation of the time evolution[1] $\rightsquigarrow$ (mixed) variational integrator[2] $\rightsquigarrow$ physical consistency with time adaptivity[3]

Introduction
Outline & overview
Problem definition
Theoretical studies
Strong forms & balances
Weak forms & balance laws
Boundary conditions
Time discrete weak forms
Time discrete operators
Time discrete balance laws
Numerical studies
Fully closed system
Fully open system
Thermally loaded system
Mechanically loaded system
Conclusions