An energy-entropy-consistent time stepping scheme for finite thermo-viscoelasticity

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

Chair of Applied Mechanics/Dynamics
Chemnitz University of Technology

March 12, 2014

[1] Chair of Computational Mechanics
University of Siegen

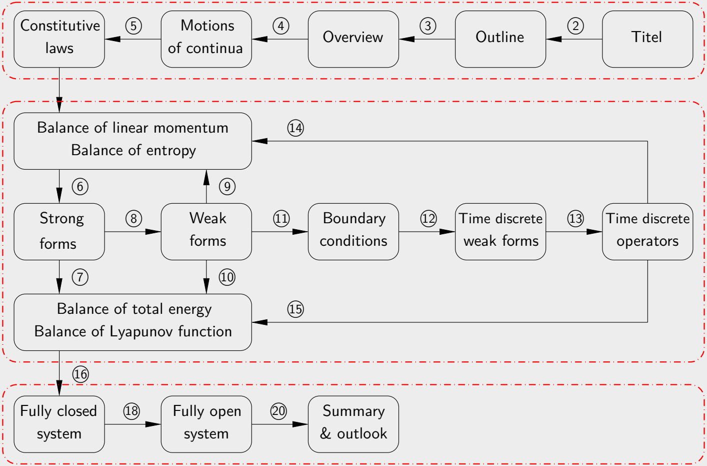
[2] Institute of Mechanics
Karlsruhe Institute of Technology

GAMM 2014 – Section S4: Structural mechanics

Acknowledgments: This research was provided by DFG grant GR 3297/2-1

Contents of the presentation

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

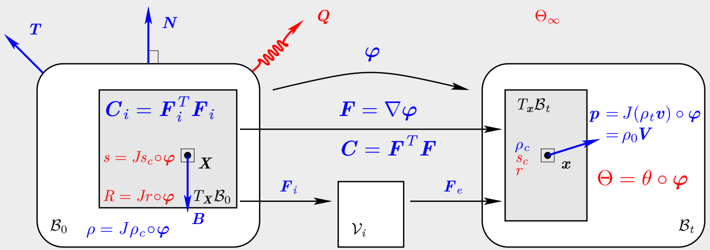
Finite element methods in time

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 of considered continuum mechanics

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

Motion of a single continuum



Energy functionals

1. Total energy, total entropy & LYAPUNOV function

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

2. Kinetic energy & internal energy

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

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]

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

Thermo-viscoelastic motion and heat conduction

1. First Piola-Kirchhoff stress tensor

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

2. Fourier's law of isotropic heat conduction

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

Dissipative behaviour

1. Total dissipation

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

2. Viscous evolution equation

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

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

Goto outline

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 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

$$\begin{aligned} \frac{\partial \boldsymbol{p}}{\partial t} &= \mathrm{Div}\,\boldsymbol{P} + \boldsymbol{B} \\ \frac{\partial \boldsymbol{\varphi}}{\partial t} &= \frac{1}{\rho}\,\boldsymbol{p} \equiv \frac{\delta H}{\delta \boldsymbol{p}} \end{aligned}$$

Heat conduction equations

1. Entropy inequality principle

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

2. Heat conduction equations

$$\begin{aligned} \frac{\partial s}{\partial t} &= \frac{1}{\Theta}\left[D^{\mathrm{vis}} + R - \mathrm{Div}\,\boldsymbol{Q}\right] \\ \Theta &= \frac{\partial e}{\partial s} \equiv \frac{\delta H}{\delta s} \end{aligned}$$

Strong forms and the first law of thermodynamics

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

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

1. Balance of mechanical energy

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

2. Balance of thermal energy

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

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

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

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

Goto outline

Weak forms derived from the strong forms

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

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)

Balance of 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 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 $\delta s(\boldsymbol{X},t) = \frac{\partial s(\boldsymbol{X},t)}{\partial t}$

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

Balance of total energy

Add balance of mechanical and thermal energy

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

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.

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

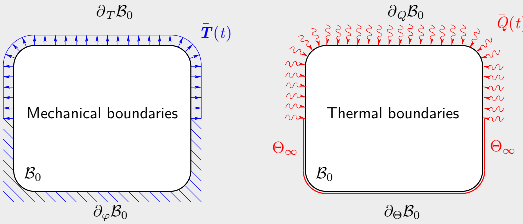
Goto outline

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]

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

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 $\quad \displaystyle\int_{\partial_\Theta \mathcal{B}_0} \delta \lambda_{n+1} \left[\Theta_{n+1} - \Theta_\infty \right] \mathrm{d}A = 0$

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]

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

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

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

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

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

Multi-variable functional (partitioned) discrete derivatives

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

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

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

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

Goto outline

Time discrete balance laws (I)

Balance of linear momentum

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

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

Balance of entropy

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

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

Balance of mechanical energy

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

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

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 $\delta\lambda_{n+1}(\boldsymbol{X}) = \lambda_{n+1}(\boldsymbol{X})$

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

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)

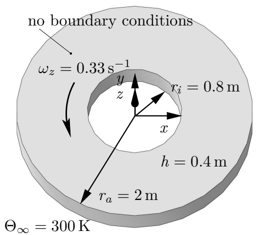
or 2. $$\frac{\Delta V}{\Delta t} = \underbrace{\frac{\Delta H}{\Delta t}}_{\text{Time discrete balance of total energy}} - \underbrace{\Theta_\infty\int_{\mathcal{B}_0}\frac{\Delta s}{\Delta t}\,\mathrm{d}V}_{\text{Time discrete balance of entropy}}$$

Goto outline

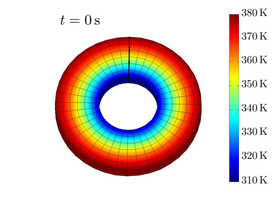
Free rotating insulated thermo-viscoelastic disc

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

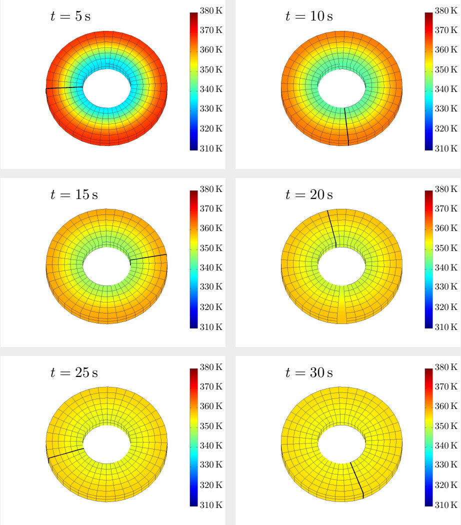
Geometry



Reference configuration

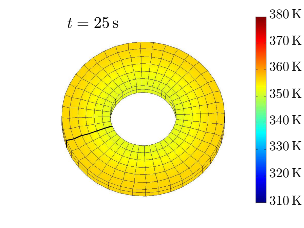


ETC integrator with $\Delta t = 0.02\,\mathrm{s}$

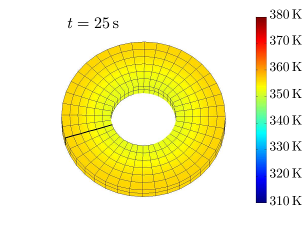


Free rotating insulated thermo-viscoelastic disc

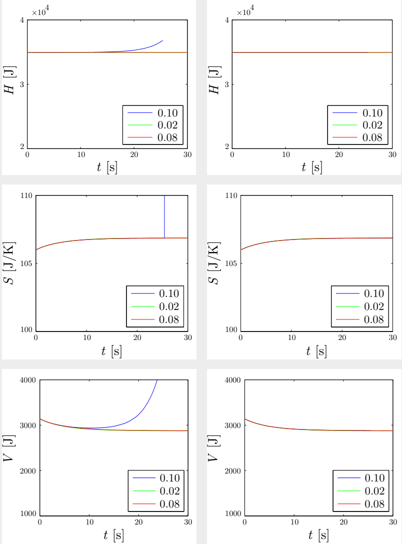
Midpoint rule ($\Delta t = 0.1\,\mathrm{s}$)



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

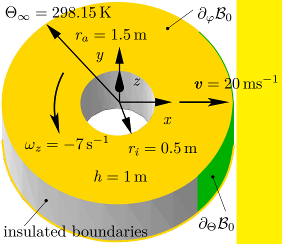


Midpoint rule ETC integrator

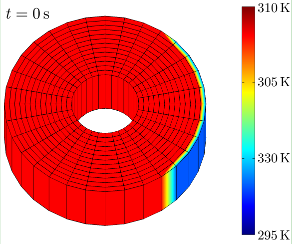


Rail-bound partly uninsulated thermo-elastic disc

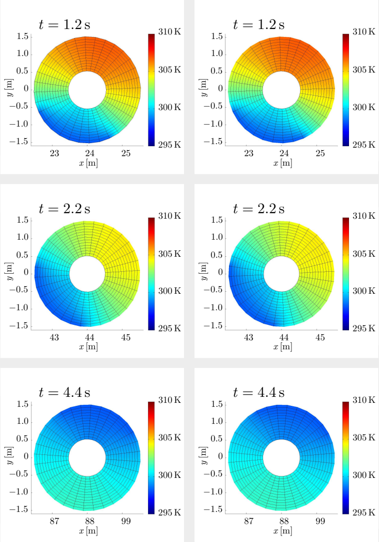
Geometry



Reference configuration

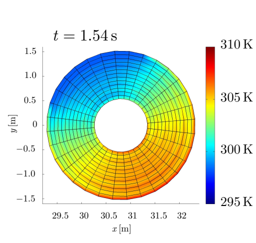


MPR ($\Delta t = 0.01\,\mathrm{s}$) ETC ($\Delta t = 0.01\,\mathrm{s}$)

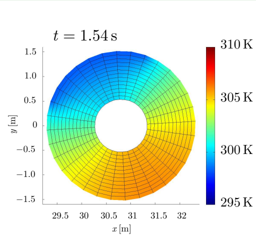


Rail-bound partly uninsulated thermo-elastic disc

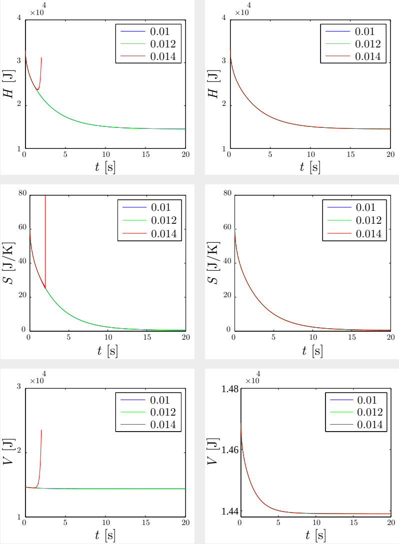
Midpoint rule ($\Delta t = 0.014\,\mathrm{s}$)



ETC integrator ($\Delta t = 0.014\,\mathrm{s}$)



Midpoint rule | ETC integrator



Summary & outlook

[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 linear momentum AND 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. Replacing Θ by thermal displacement $\partial_t \alpha$ in the weak formulation[1]
   $\rightsquigarrow$ mixed variational integrator[2] $\rightsquigarrow$ physical consistency with time adaptivity[3]

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