Physically consistent simulation of technical polymers

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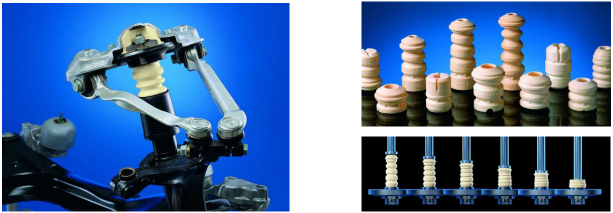
November 26, 2011

18th Bohemian-Saxon-Silesian Mechanics Colloquium

TU-Bergakademie Freiberg

Unfilled/Filled polymers

❶ Unfilled elastomers



Elastomer springs by BASF Polyurethanes GmbH

❷ Filled conductive polymers

Heat sinks and coil bodies by CoolPoly, k=1,...,10 W/mK, $\rho > 1$ TΩ cm, $\rho_0 = 1.47$ g/cm^3

Challenges of numerical simulation methods

[1] Lion [1997], Reese & Govindjee [1998], Ehlers & Markert [2000], Miehe & Keck [2000], Haupt & Sedlan [2001], Rieger [2004], Kleuter [2007], Dal & Kaliske [2009], Méndez Diez [2010]

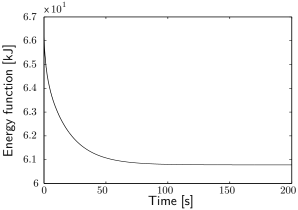
[2] Simo et al. [1993], Ellsiepen [1999], Kirchner & Simeon [1999], Reese & Wriggers [1999], Doll et al. [2000], Hartmann [2003], Reese et. al [2005], Bischoff & Romero [2006]

① Realistic results

- Validated material laws[1]
- Identified material param.[1]
- Validated boundary cond.[1]

- Locking-free space mesh[2]
- Momentum consistent &
- Energy consistent time mesh

Rotating heat pipe (McMaster University, Ca)



Energy balance relative to equilibrium

② Efficient methods

- Numerical stability

  ⇝ coarse space-time meshes

- Variable accuracy[2]

  ⇝ adaptive space-time meshing

Dynamics of solids

Oden [1972], Gurtin [1981], Miehe [1988], Holzapfel [2000], Andrews [2005], Chernyshev [2007], Fernández & Kuttler [2010]

1. Lagrangian local momentum balance

$$\boldsymbol{v}_t := \frac{\partial \boldsymbol{\varphi}_t}{\partial t} \qquad \boxed{\frac{\partial \boldsymbol{v}_t}{\partial t} = \frac{1}{\rho_0}\,\mathrm{D{\small IV}}[\boldsymbol{F}_t \boldsymbol{S}_t] + \boldsymbol{b}_t}$$

2. Deformation gradient/metric & strain measure

$$\boldsymbol{F}_t := \mathrm{G{\small RAD}}[\boldsymbol{\varphi}_t] \qquad \boldsymbol{C}_t := [\boldsymbol{F}_t^\flat]^T \boldsymbol{F}_t \qquad \boldsymbol{E}_t := \frac{1}{2}\,[\boldsymbol{C}_t - \boldsymbol{I}]$$

3. Piola/Mandel stress tensor

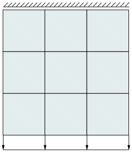
$$\boldsymbol{S}_t := 2\,\frac{\partial \psi_t}{\partial \boldsymbol{C}} \qquad \boldsymbol{\Sigma}_t^\flat := \boldsymbol{C}_t \boldsymbol{S}_t$$

4. Stress power & deformation rate tensor

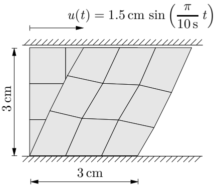
$$\mathcal{P}_t := \boldsymbol{\Sigma}_t^\flat : \boldsymbol{L}_t^\sharp \qquad \boldsymbol{L}_t^\sharp := \frac{1}{2}\,\boldsymbol{C}_t^{-1}\,\frac{\partial \boldsymbol{C}}{\partial t}$$

Behaviour of viscoelastic elastomers

Miehe [1988], van den Bogert & de Borst [1994], Holzapfel & Simo[1996], Holzapfel[1996], Lion [1997], Reese & Govindjee [1998], Haupt [2002], Takács [2003]

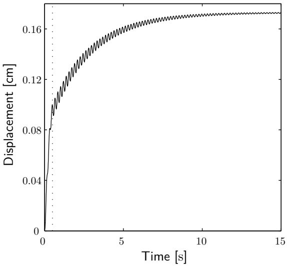


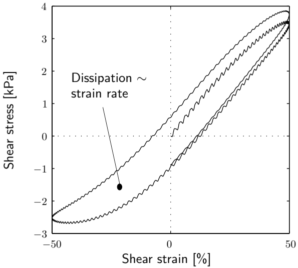
$$-F_y(t) = \begin{cases} 4\,\dfrac{\mathrm{kN}}{\mathrm{cm}}\,\sin\left(\dfrac{\pi}{\mathrm{s}}\,t\right) & \text{für} \quad 0\,\mathrm{s} \leqslant t \leqslant 0.5\,\mathrm{s} \\ 4\,\dfrac{\mathrm{kN}}{\mathrm{cm}} & \text{für} \quad 0.5\,\mathrm{s} \leqslant t \leqslant 15\,\mathrm{s} \end{cases}$$



$$\boldsymbol{S}_t = \boldsymbol{f}(\boldsymbol{E}_t) + \underset{\substack{0\leqslant\sigma\leqslant s_\tau\\ 0\leqslant\tau\leqslant t}}{\mathfrak{F}}\,[\hat{\boldsymbol{E}}_\sigma \circ s_\tau]$$

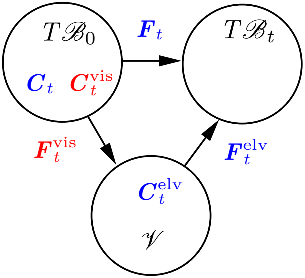
$$s_\tau = \int_0^\tau \|\dot{\boldsymbol{E}}(t)\|\,\mathrm{d}t$$ (curve parameter of hysteresis)





Viscous evolution of isotropic elastomers

Miehe[1988], Le Tallec et al. [1993], Kaliske [1995], Reese & Govindjee [1998], Reese [2001], Kleuter [2007], Hartmann & Hamkar [2010]



① Elastic metric tensor

$$\boldsymbol{C}_t^{\mathrm{elv}} := [\boldsymbol{F}_t^{\mathrm{vis}}]^{-T}\,\boldsymbol{C}_t[\boldsymbol{F}_t^{\mathrm{vis}}]^{-1}$$

② Elastic invariants

$$\mathfrak{I}(\boldsymbol{C}_t^{\mathrm{elv}}) = \mathfrak{I}(\boldsymbol{C}_t\,[\boldsymbol{C}_t^{\mathrm{vis}}]^{-1})$$

③ Viscous internal variable

$$\boldsymbol{C}_t^{\mathrm{vis}} := [\boldsymbol{F}_t^{\mathrm{vis},\flat}]^T\,\boldsymbol{F}_t^{\mathrm{vis}}$$

④ Viscous evolution equation

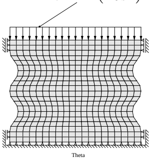
$$\boxed{\boldsymbol{\Sigma}_t^{\flat} = n_{\mathrm{dim}}\,V_{\mathrm{sph}}\,\textsc{Sph}([\boldsymbol{L}_t^{\mathrm{vis},\sharp}]^T) + 2\,V_{\mathrm{dev}}\,\textsc{Dev}([\boldsymbol{L}_t^{\mathrm{vis},\sharp}]^T)}$$

⑤ Viscous Dissipation/rate tensor

$$D_t^{\mathrm{vis}} := \boldsymbol{\Sigma}_t^{\flat} : \boldsymbol{L}_t^{\mathrm{vis},\sharp} \geqslant 0 \qquad \boldsymbol{L}_t^{\mathrm{vis},\sharp} := \frac{1}{2}\,[\boldsymbol{C}_t^{\mathrm{vis}}]^{-1}\,\frac{\partial \boldsymbol{C}^{\mathrm{vis}}}{\partial t}$$

Tension/Pressure of an elastomer spring (VE)

$$-F_y(t) = 30\,\frac{\mathrm{kN}}{\mathrm{cm}}\,\sin\left(\frac{2\,\pi}{1.6\,\mathrm{s}}\,t\right)$$



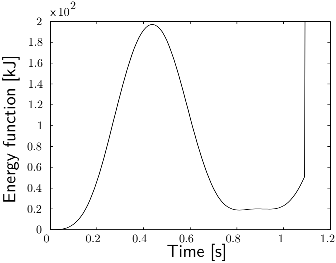
Height	H	$10\,\mathrm{cm}$
Width	W	$12.82\,\mathrm{cm}$
Viscoelastic Simo-Taylor material		
Mass density	ρ_0	$10\,\mathrm{kg/cm^2}$
First Lamé constant	μ	$7.5\,\mathrm{kJ/cm^2}$
Second Lamé constant	λ	$30\,\mathrm{kJ/cm^2}$
Deviatoric viscosity	V_{dev}	$10\,\mathrm{kJs/cm^2}$
Spherical viscosity	V_{sph}	$50\,\mathrm{kJs/cm^2}$
Time step size	h_n	$10\,\mathrm{ms}$
Global iteration tolerance	tol	$10^{-6}\,\mathrm{J}$
Local iteration tolerance	tolevo	$10^{-9}\,\mathrm{J/cm^2}$
Number of spatial elements	n_{el}	400
Number of spatial nodes	n_{no}	441

Midpoint rule $(h_n = 10\,\mathrm{ms},\, T = 1.15\,\mathrm{s})$

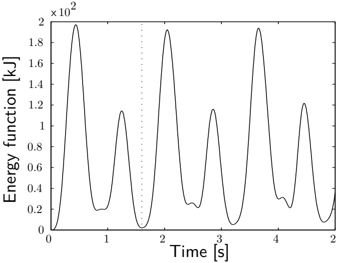
eG method $(h_n = 10\,\mathrm{ms},\, T = 5\,\mathrm{s})$

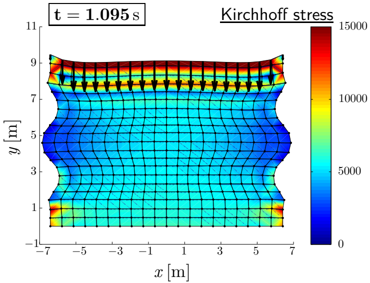
Energy-Time behaviour & Stress distribution

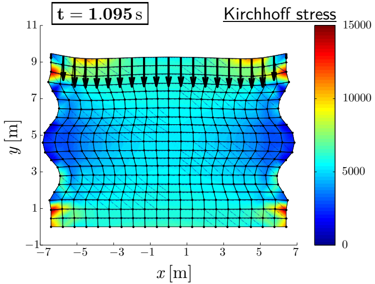
Midpoint rule



eG method







Thermodynamics of elastomers

Oden [1972], Miehe [1988], Holzapfel & Simo [1996], Bérardi et al. [1996], Lion [1997], Reese [2000], Boukamel et al. [2001]

1. Lagrangian local entropy balance

$$\eta_t := -\frac{\partial \psi_t}{\partial \theta} \qquad \boxed{\frac{\partial \eta_t}{\partial t} = -\frac{1}{\theta_t}\,\mathrm{D{\small IV}}[\boldsymbol{Q}_t] + \frac{D_t^{\mathrm{vis}}}{\theta_t} + \frac{r_t}{\theta_t}}$$

2. Fourierian isotropic heat flux

$$\boldsymbol{q}_t := -k_0\,(J_t\,\boldsymbol{F}_t^{\sharp})^{-T}\,\mathrm{G{\small RAD}}[\theta_t] \qquad \boldsymbol{Q}_t := J_t\,\boldsymbol{F}_t^{-1}\,\boldsymbol{q}_t$$

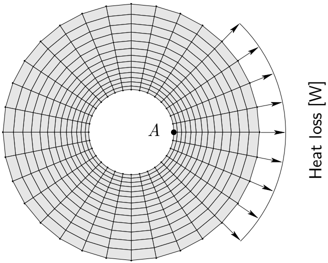
3. Specific heat capacity & thermal expansion

$$\theta_t\,\frac{\partial \eta_t}{\partial \theta} =: c \geq 0 \qquad \frac{1}{n_{\mathrm{dim}}}\,\frac{\partial \mathrm{D{\small ET}}[\boldsymbol{F}_t]}{\partial \theta} =: \beta \geq 0$$

4. Thermal dissipation

$$D_t^{\mathrm{cdu}} := -\mathrm{G{\small RAD}}[\ln \theta_t] \cdot \boldsymbol{Q}_t \geq 0$$

Cooling of an elastomer spring (TE)

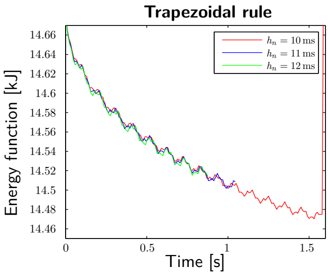


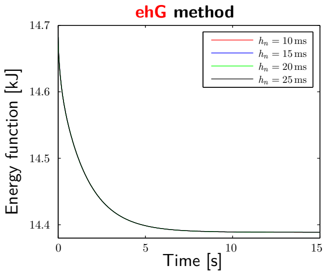
Inner radius	R_i	$0.5\,\mathrm{m}$
Outer radius	R_a	$1.5\,\mathrm{m}$
Thermoelastic Simo-Taylor material		
Mass density	ρ_0	$10\,\mathrm{kg/m^2}$
First Lamé constant	μ	$7.5\,\mathrm{kJ/m^2}$
Second Lamé constant	λ	$30\,\mathrm{kJ/m^2}$
Specific heat capacity	c	$0.3\,\mathrm{kJ/m^2K}$
Heat expansion coefficient	β	$10^{-4}\,\mathrm{K}^{-1}$
Heat conduction coefficient	k_0	$0.3\,\mathrm{kW/K}$
Ambient temperature	Θ_∞	$298.15\,\mathrm{K}$
Global iteration tolerance	tol	$10^{-6}\,\mathrm{J}$
Number of spatial elements	n_{el}	416
Number of spatial nodes	n_{no}	448

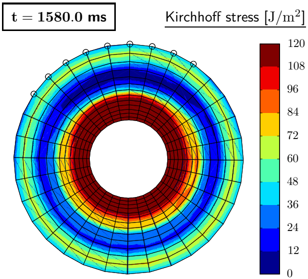
Trapezoidal rule $(h_n = 10\,\mathrm{ms},\ T = 1.59\,\mathrm{s})$

ehG method $(h_n = 25\,\mathrm{ms},\ T = 15\,\mathrm{s})$

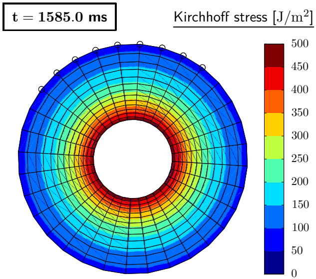
Energy-time behaviour & Stress distribution





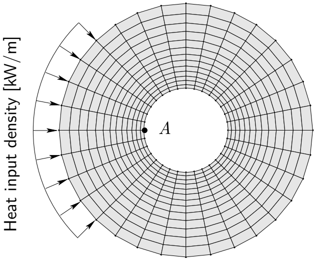


$h_n = 10$ ms



$h_n = 10$ ms

Heating of an elastomer spring (TE)

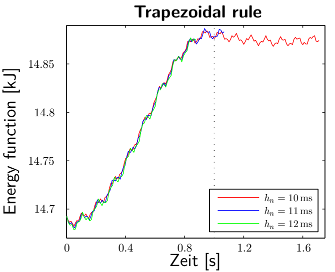


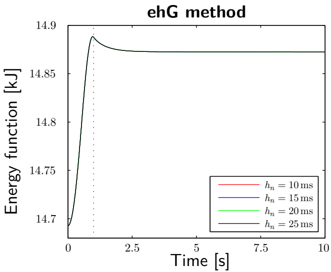
Inner radius	R_i	$0.5\,\mathrm{m}$
Outer radius	R_a	$1.5\,\mathrm{m}$
Thermoelastic Simo-Taylor material		
Mass density	ρ_0	$10\,\mathrm{kg/m^2}$
First Lamé constant	μ	$7.5\,\mathrm{kJ/m^2}$
Second Lamé constant	λ	$30\,\mathrm{kJ/m^2}$
Specific heat capacity	c	$0.3\,\mathrm{kJ/m^2K}$
Heat expansion coefficient	β	$10^{-4}\,\mathrm{K}^{-1}$
Heat conduction coefficient	k_0	$0.3\,\mathrm{kW/K}$
Ambient temperature	Θ_∞	$298.15\,\mathrm{K}$
Global iteration tolerance	tol	$10^{-6}\,\mathrm{J}$
Number of spatial elements	n_{el}	416
Number of spatial nodes	n_{no}	448

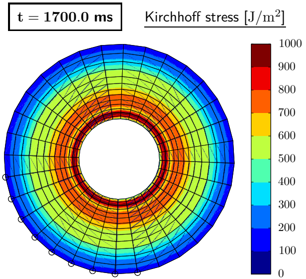
Trapezoidal rule $(h_n = 10\,\mathrm{ms},\ T = 1.71\,\mathrm{s})$

ehG method $(h_n = 25\,\mathrm{ms},\ T = 10\,\mathrm{s})$

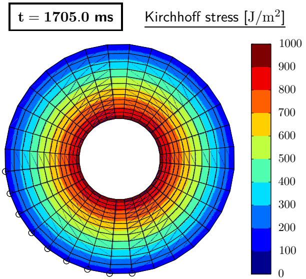
Energy-Time behaviour & Stress distribution







$h_n = 10$ ms



$h_n = 10$ ms

Energy-consistent finite element method

Argyris & Scharpf [1969], Hughes et al. [1978], Betsch & Steinmann [2001], Hansbo [2001], Cockburn [2003], Bui [2007]

❶ Relative total energy

$$
\mathcal{V}(t) = \int_{\mathscr{B}_0} \rho_0 \boldsymbol{v}_t \cdot \boldsymbol{v}_t + \psi_t + (\theta_t - \theta_\infty)\,\eta_t
$$

❷ Energy-consistent finite element method

$$
\begin{aligned}
\mathcal{V}(T)-\mathcal{V}(t_0) = {} & \begin{aligned}[t]
& \int_{\mathscr{T}}\int_{\mathscr{B}_0} \rho_0 \boldsymbol{v}_t \cdot \frac{\partial \boldsymbol{v}_t}{\partial t} \\
+ & \int_{\mathscr{T}}\int_{\mathscr{B}_0} \frac{\partial \psi_t}{\partial \boldsymbol{F}} : \frac{\partial \boldsymbol{F}_t}{\partial t} \\
+ & \int_{\mathscr{T}}\int_{\mathscr{B}_0} \frac{\partial \psi_t}{\partial \boldsymbol{C}^{\mathrm{vis}}} : \frac{\partial \boldsymbol{C}_t^{\mathrm{vis}}}{\partial t} \\
+ & \int_{\mathscr{T}}\int_{\mathscr{B}_0} (\theta_t - \theta_\infty)\,\frac{\partial \eta_t}{\partial t}
\end{aligned}
\underbrace{\begin{aligned}[t]
& + \int_{\mathscr{T}}\int_{\mathscr{B}_0} \rho_0 \frac{\partial \boldsymbol{v}_t}{\partial t} \cdot \left[\frac{\partial \boldsymbol{\varphi}_t}{\partial t} - \boldsymbol{v}_t\right] \\
& - \int_{\mathscr{T}}\int_{\mathscr{B}_0} \frac{\partial \boldsymbol{\varphi}_t}{\partial t} \cdot \left[\rho_0 \frac{\partial \boldsymbol{v}_t}{\partial t} - \mathrm{D{\scriptstyle IV}}[\boldsymbol{F}_t \boldsymbol{S}_t]\right] \\
& + \int_{\mathscr{T}}\int_{\mathscr{B}_0} \frac{\partial \boldsymbol{C}^{\mathrm{vis}}}{\partial t} : \left[\frac{1}{2}[\boldsymbol{C}_t^{\mathrm{vis}}]^{-1}\boldsymbol{\Sigma}_t - \boldsymbol{Y}_t\right] \\
& - \int_{\mathscr{T}}\int_{\mathscr{B}_0} (\theta_t - \theta_\infty) \left[\frac{\partial \eta_t}{\partial t} + \frac{1}{\theta_t}\,\mathrm{D{\scriptstyle IV}}[\boldsymbol{Q}_t] - \frac{D_t^{\mathrm{vis}}}{\theta_t}\right] \\
& + \int_{\mathscr{T}}\int_{\mathscr{B}_0} \frac{\partial \theta_t}{\partial t} \left[\frac{\partial \psi_t}{\partial \theta_t} + \eta_t\right] \\
& - \int_{\mathscr{T}}\int_{\mathscr{B}_0} \frac{\partial \boldsymbol{F}_t}{\partial t} : \left[\frac{\partial \psi_t}{\partial \boldsymbol{F}_t} - \boldsymbol{F}_t \boldsymbol{S}_t\right]
\end{aligned}}_{0} \\
= {} & - \int_{\mathscr{T}}\int_{\mathscr{B}_0} \frac{\theta_\infty}{\theta_t} D_t^{\mathrm{tot}} \leqslant 0
\end{aligned}
$$

Discrete energy-consistent approximations

Gonzalez [1996], Armero & Romero [2001], Betsch & Steinmann [2001], Wriggers [2001], Kübler et al. [2003], Sansour et al. [2004], Bargmann [2006], Mohr et al. [2008]

1. Discrete Galerkin methods
    - Standard continuous Galerkin method where the test function is a time derivative
    - Non-standard discontinuous Galerkin method with a special jump term elsewhere.
2. Non-standard approximation of the deformation metric
3. Non-standard approximation of the Mandel stress tensor

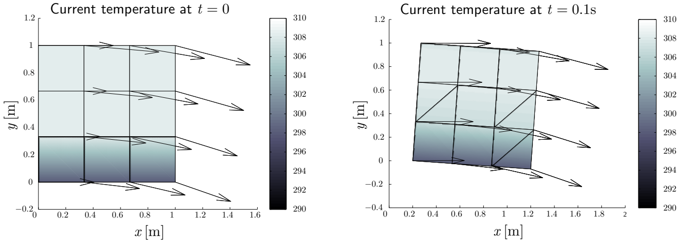
$$\boldsymbol{\Sigma}_{\alpha}^{\mathrm{num},\flat} := \overline{\boldsymbol{\Sigma}}_{\alpha}^{\flat} + \overline{\boldsymbol{M}}_{\alpha}^{\flat} + \overline{\boldsymbol{\Sigma}}_{\alpha}^{\mathrm{dam},\flat} + \overline{\boldsymbol{M}}_{\alpha}^{\mathrm{dam},\flat}$$

4. Non-standard approximation of the entropy
5. Viscous damping

$$\overline{\boldsymbol{\Sigma}}_{\alpha}^{\mathrm{dam},\flat} := \frac{\overline{J}_{\alpha}}{h_n} \left\{ n_{\mathrm{dim}}\, D_{\mathrm{sph}}\, \textsc{Sph}(\overline{\boldsymbol{L}}_{\alpha}^{\sharp})^{T} + 2\, D_{\mathrm{dev}}\, \textsc{Dev}(\overline{\boldsymbol{L}}_{\alpha}^{\sharp})^{T} \right\}$$

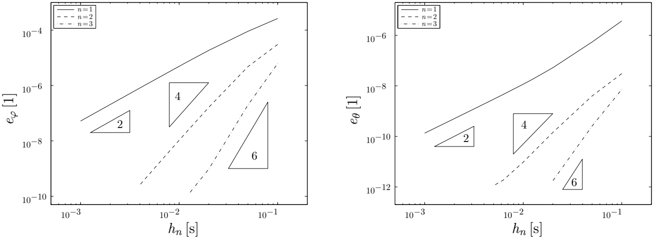
Accuracy order of the energy-based integrator

1 Free flying thermo-viscoelastic elastomer plate


Current temperature at $t = 0$

Current temperature at $t = 0.1\text{s}$

2 Relative error of position and temperature



Tension/Pressure of an elastomer spring (TVE)

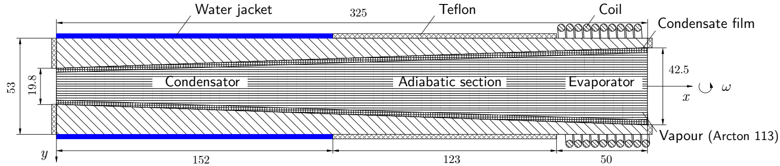
Temperature distribution of the ehG method $(h_n = 10\,\mathrm{ms},\, T = 5\,\mathrm{s})$

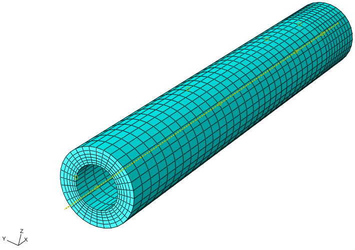
Tension/Pressure of an elastomer spring (TVE)

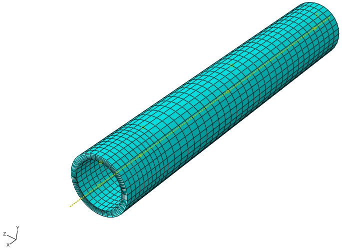
Stress distribution of the ehG method $(h_n = 10\,\mathrm{ms},\, T = 5\,\mathrm{s})$

Simulation of a rotating TVPE heat pipe

Daniels & Al-Jumaily [1974], Li et al. [1993], Harley & Faghri [1995], Streby & Ponnappan [1996], Song et al. [2003,2004,2008], Shukla et al. [2009]
Reich & Beer [1989], Reich et al. [1989], Weigand & Beer [1989,1992], Weigand [2004]







	Condensator	Adiabatic section	Evaporator
Outside	$\theta = \theta_\infty$ (Controlling)	$\overline{Q} = 0$	Convection & Radiation
Inside	Convection & Pressure	Convection & Pressure	Convection & Pressure

Mechanical and thermal boundary conditions

Daniels & Al-Jumaily [1974], Harley & Faghri [1995], Baehr & Stephan [1996], Bay et al. [2003]

1. Inside pressure by gas expansion & radial acceleration

$$p = \rho_v \left\{ \frac{R\, T_v}{M_v} + \frac{\omega^2 r^2}{2} \right\}$$

2. Convection on the condenser & adiabatic section

$$\overline{Q}_c = h_c\, A_c\, (T_s - \theta_c) \qquad \overline{Q}_a = h_a\, A_a\, (T_s - \theta_a)$$

3. Convection on the evaporator

$$\overline{Q}_e = h_e\, A_e\, (\theta_e - T_s) \qquad \overline{Q}_v = \alpha_v\, (\theta_e - \theta_\infty)$$

4. Heat radiation/input of the evaporator

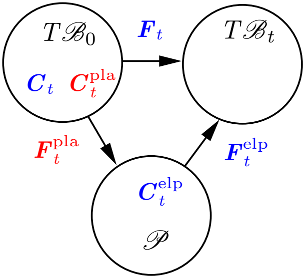
$$\overline{Q}_v = \epsilon_e\, \sigma\, (\theta^4 - \theta_\infty^4) \qquad r_e = \frac{Q_{\mathrm{inp}}}{V_e}$$

5. Experimental data from the literature

Vapour (Ideal gas)	$\rho_v = 2.605\mathrm{kg/m^3}$ $T_v = 346\mathrm{K}$ $M_v = 0.18738\mathrm{kg/mol}$		
Condensate film	$T_s = 106°\mathrm{C}$		
	Condensator	Adiabatic section	Evaporator
Inside	$h_c = 483\mathrm{W/m^2K}$	$h_a = h_c$	$h_e = 4438\mathrm{W/m^2K}$
Outside			$\alpha_v = 13.566\mathrm{W/m^2K}$ $\epsilon_e = 0.92$

Plastic evolution equation of filled polymers

James & Green [1975], Bigg [1986], Heinle & Drummer [2010], Egelkraut et al. [2008]
Lion [1996], Miehe & Keck [2000], Haupt & Sedlan [2001], Haupt [2002], Hartmann & Neff [2003],Hartmann [2010]



❶ Plastic internal variable

$$\mathbf{C}^{\rm pla}_t := [\mathbf{F}^{{\rm pla},\flat}_t]^T\,\mathbf{F}^{\rm pla}_t$$

❷ Plastic dissipation

$$D^{\rm pla}_t := \boldsymbol{\Sigma}^\flat_t : \mathbf{L}^{{\rm pla},\sharp}_t \geqslant 0$$

❸ Plastic rate tensor

$$\mathbf{L}^{{\rm pla},\sharp}_t := \frac{1}{2}\,[\mathbf{C}^{\rm pla}_t]^{-1}\,\frac{\partial\mathbf{C}^{\rm pla}}{\partial t}$$

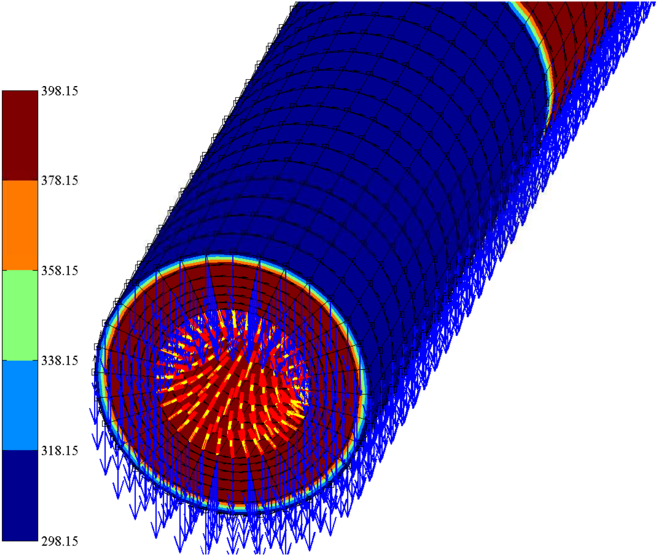
❹ Plastic evolution equation

$$\boxed{\boldsymbol{\Sigma}^\flat_t = n_{\rm dim}\,V_{\rm sph}\,\textsc{Sph}([\hat{\mathbf{L}}^{{\rm pla},\sharp}_t]^T) + 2\,V_{\rm dev}\,\textsc{Dev}([\hat{\mathbf{L}}^{{\rm pla},\sharp}_t]^T)}$$

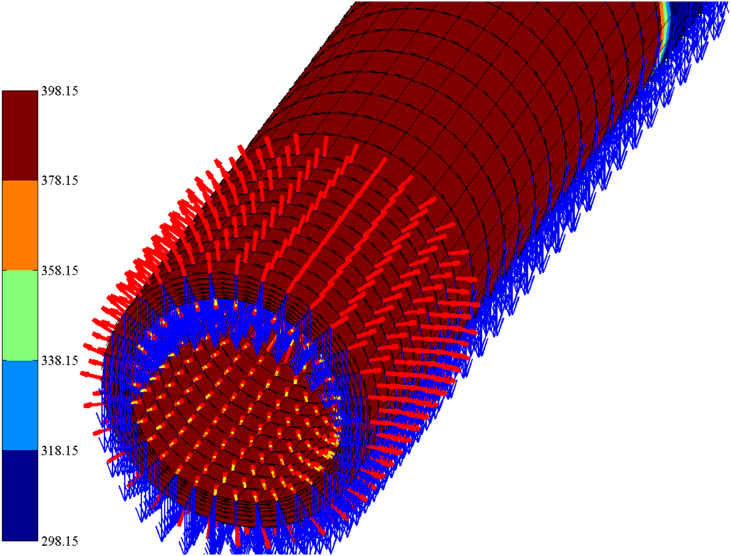
❺ Plastic evolution tensor

$$\hat{\mathbf{L}}^{{\rm pla},\sharp}_t := \frac{1}{2}\,[\mathbf{C}^{\rm pla}_t]^{-1}\,\frac{\partial\mathbf{C}^{\rm pla}_t}{\partial s} = \frac{1}{\|\dot{\mathbf{E}}\|}\,\mathbf{L}^{{\rm pla},\sharp}_t$$

Condensator section of the heat pipe



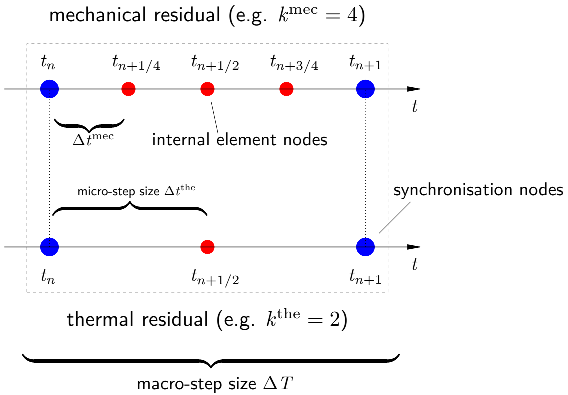
Evaporator section of the heat pipe



Closing remarks: multiscale in time

Hughes & Stewart [1996], Bottasso[2002], Ladevèze & Nouy [2003], Kassiotis, Colliat, Ibrahimbegovic & Matthies [2009], Takizawa & Tezduyar [2011]

1. Advantages of the ehG method
   - energy-momentum consitency
   - higher-order accuracy
   - multiscale approximation (1st step towards p-adaptivity)
2. Thermo-mechanical multiscale approximation



mechanical residual (e.g. $k^{\mathrm{mec}} = 4$)

thermal residual (e.g. $k^{\mathrm{the}} = 2$)

macro-step size ΔT