Coupled Temperature-Deformation Computations for Viscoelastic Materials with Fractional Derivatives

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Outline

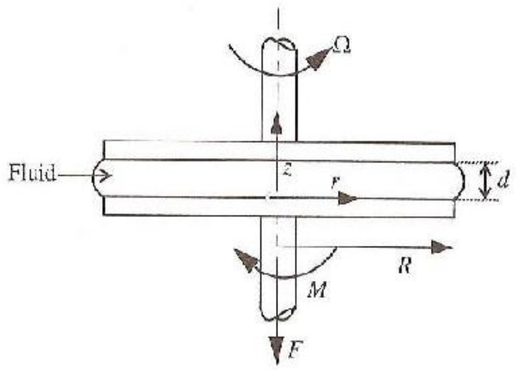
- Motivation
- Balance of momentum
- Balance of energy
- Material relations
- Numerical procedure
- Results
- Outlook

Motivation

- Viscoelastic materials
  - both viscous and elastic characteristics
  - strain rate dependence
- e.g. Polycarbonate melts
- Aim is to study deformation behaviour

Experiment

- Test conducted using parallel plate viscometer



- 2 parallel plates
- Input: Upper plate rotation
- Output: Torque to keep the lower plate stationary

Balance of Momentum

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_B \rho v_i dV = \int_{\partial B} n_j \sigma_{ji} \mathrm{d}a + \int_B \rho f_i \mathrm{d}V$$

Changing to material frame:

$$\int_{B_0} \left(\frac{1}{\Delta t \Delta t} \rho_0 \left(u_i - 2u_i^0 + u_i^{00} \right) - \frac{\partial}{\partial X_r} \left(\sigma_{ji} \left(F^{-1} \right)_{jr} J \right) \right) \delta u_i \, \mathrm{d}V_0$$

$$\left(F^{-1} \right)_{jr} = \frac{\partial X_j}{\partial x_r}$$

δu_i is the trial function

Balance of Energy

$$\frac{\mathrm{d}}{\mathrm{d}\,t}\int_B \left(\rho u + \frac{\rho}{2} v_i v_i \right) \mathrm{d}V = -\int_{\partial B} q_i n_i \,\mathrm{d}\,A + \int_{\partial B} \sigma_{ji} v_i n_j \,\mathrm{dA} + \int_B \rho r \,\mathrm{d}V + \int_B \rho f_i v_i \,\mathrm{d}V$$

Changing to material frame:

$$\int_{B_0} \left(\rho_0 \boxed{\frac{\partial u}{\partial t}} + \frac{\partial \boxed{Q_r}}{\partial X_r} - \boxed{\sigma_{ji}} (F^{-1})_{rj} J \frac{\partial v_i}{\partial X_r} \right) \delta T \,\mathrm{d}V_0 = 0$$

u is the specific internal energy

$$Q_r = -\kappa \delta_{rj} \frac{\partial T}{\partial X_j} \rightarrow \text{(Fourier's Law)}$$

Constitutive Relation

- Fractional Zener model*:

$$\sigma_{ij} + \tau_0^\alpha \frac{\mathrm{d}^\alpha \sigma_{ij}}{\mathrm{d}t^\alpha} = G_e \left(\varepsilon_{ij} + \tau_0^\alpha \frac{\mathrm{d}^\alpha \varepsilon_{ij}}{\mathrm{d}t^\alpha} \right) + G_0 \tau_0^\beta \frac{\mathrm{d}^\beta \varepsilon_{ij}}{\mathrm{d}t^\beta}$$

Where G_e ,G_o, τ_0,α and β are material parameters

$$\sigma_{ij}^R = G_e \varepsilon_{ij}$$

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Friedrich, C. , Mechanical stress relaxation in polymers: fractional integral model versus fractional differential model
Journal of Non-Newtonian Fluid Mechanics, **1993**, *46*, 307 - 314

Bagley, R. L. & Torvik, P. J., On the Fractional Calculus Model of Viscoelastic Behavior
Journal of Rheology, SOR, **1986**, *30*, 133-155

Internal Energy

$$\mathrm{d}U = \mathrm{d}Q + \mathrm{d}W$$

$$\mathrm{d}U = T\mathrm{d}S + \sigma_{ij}^{R}\mathrm{d}\varepsilon_{ij}$$

$$\dot{U} = T\dot{S} + \sigma_{ij}^{R}\dot{\varepsilon}_{ij}$$

$$\rho_0\dot{u} = T\dot{S} + \sigma_{ij}^{R}\dot{\varepsilon}_{ij}$$

Internal Energy

$$u = u(\varepsilon_{kl}, T) \qquad \sigma_{ij}^R = \sigma_{ij}^R(\varepsilon_{kl}, T), \quad S = S(\varepsilon_{kl}, T)$$

$$\mathrm{d}\sigma_{ij}^R = \underbrace{\left.\frac{\partial \sigma_{ij}^R}{\partial \varepsilon_{kl}}\right|_T}_{?} \mathrm{d}\varepsilon_{kl} + \underbrace{\left.\frac{\partial \sigma_{ij}^R}{\partial T}\right|_{\varepsilon_{kl}}}_{?} \mathrm{d}T$$

$$\mathrm{d}S = \underbrace{\left.\frac{\partial S}{\partial \varepsilon_{kl}}\right|_T}_{?} \mathrm{d}\varepsilon_{kl} + \underbrace{\left.\frac{\partial S}{\partial T}\right|_{\varepsilon_{kl}}}_{?} \mathrm{d}T$$

Internal Energy

$$u = u(\varepsilon_{kl}, T) \qquad \sigma_{ij}^{R} = \sigma_{ij}^{R}(\varepsilon_{kl}, T)\,, \quad S = S(\varepsilon_{kl}, T)$$

$$\mathrm{d}\sigma_{ij}^{R} = \underbrace{\left.\frac{\partial \sigma_{ij}^{R}}{\partial \varepsilon_{kl}}\right|_{T}} \mathrm{d}\varepsilon_{kl} \quad + \quad \underbrace{\left.\frac{\partial \sigma_{ij}^{R}}{\partial T}\right|_{\varepsilon_{kl}}} \mathrm{d}T$$

$$C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \qquad p_{ij} = p\delta_{ij}$$

$$\mathrm{d}S = \underbrace{\left.\frac{\partial S}{\partial \varepsilon_{kl}}\right|_{T}}_{?} \mathrm{d}\varepsilon_{kl} + \underbrace{\left.\frac{\partial S}{\partial T}\right|_{\varepsilon_{kl}}}_{?} \mathrm{d}T$$

Internal Energy

$$T\,\mathrm{d}S = \underbrace{T\left.\frac{\partial S}{\partial \varepsilon_{kl}}\right|_{T}}_{\text{Heat of Deformation}}\mathrm{d}\varepsilon_{kl} + \underbrace{T\left.\frac{\partial S}{\partial T}\right|_{\varepsilon_{kl}}}_{\text{Heat capacity at constant strain}}\mathrm{d}T$$

$$\left.\frac{\partial S}{\partial T}\right|_{\varepsilon_{ij}} = \frac{C_{\varepsilon}}{T}$$

$$\psi = U - TS$$

$$\mathrm{d}\psi = \mathrm{d}U - T\mathrm{d}S - S\mathrm{dT}$$

$$\mathrm{d}\psi = \sigma_{ij}^{R}\mathrm{d}\varepsilon_{ij} - S\mathrm{d}T \quad , \quad \psi = \psi\left(\varepsilon_{ij}, T\right)$$

$$\left.\frac{\partial\psi}{\partial\varepsilon_{ij}}\right|_{T} = \sigma_{ij}^{R} \quad , \quad \left.\frac{\partial\psi}{\partial T}\right|_{\varepsilon_{ij}} = -S$$

$$\frac{\partial^2\psi}{\partial T\partial\varepsilon_{ij}} = \frac{\partial^2\psi}{\partial\varepsilon_{ij}\partial T}$$

$$\Rightarrow \frac{\partial\sigma_{ij}^{R}}{\partial T} = -\frac{\partial S}{\partial\varepsilon_{ij}}$$

Internal Energy

$$\frac{\partial S}{\partial \varepsilon_{ij}} = -\frac{\partial \sigma_{ij}^R}{\partial T} = -\frac{\partial \sigma_{ij}^R}{\partial \varepsilon_{kl}} \frac{\partial \varepsilon_{kl}}{\partial T} \quad , \quad \frac{\partial \varepsilon_{kl}}{\partial T} = \underbrace{\alpha_{kl} = \alpha \delta_{kl}}$$

Coefficients of thermal expansion

$$\frac{\partial \sigma_{ij}^R}{\partial \varepsilon_{kl}} \frac{\partial \varepsilon_{kl}}{\partial T} = \left(\lambda \delta_{ij} \delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\right)\left(\alpha \delta_{kl}\right)$$

$$= (3\lambda + 2\mu)\alpha \delta_{ij}$$

$$= 2\mu\alpha\delta_{ij} = G_e \alpha \delta_{ij} \ , \qquad \sigma_{ij}^R = G_e \varepsilon_{ij}$$

For no volume change, $\lambda = 0$

Internal Energy

$$\rho_0 \dot{u} = T\dot{S} + \sigma_{ij}^R \dot{\varepsilon}_{ij}$$

$$\mathrm{d}\sigma_{ij}^R = \left.\frac{\partial \sigma_{ij}^R}{\partial \varepsilon_{kl}}\right|_T \mathrm{d}\varepsilon_{kl} + \left.\frac{\partial \sigma_{ij}^R}{\partial T}\right|_{\varepsilon_{kl}} \mathrm{d}T$$

$$\mathrm{d}S = \left.\frac{\partial S}{\partial \varepsilon_{kl}}\right|_T \mathrm{d}\varepsilon_{kl} + \left.\frac{\partial S}{\partial T}\right|_{\varepsilon_{kl}} \mathrm{d}T$$

Internal Energy

$$\rho_0 \dot{u} = T\dot{S} + \sigma_{ij}^R \dot{\varepsilon}_{ij}$$

$$\mathrm{d}\sigma_{ij}^R = G_e \,\mathrm{d}\,\varepsilon_{ij} + G_e \alpha \delta_{ij} \,\mathrm{d}\,T$$

$$\mathrm{d}S = -G_e \alpha \delta_{ij} \,\mathrm{d}\,\varepsilon_{ij} + \frac{C_\varepsilon}{T} \mathrm{d}\,T$$

$$\boxed{\rho_0 \dot{u} = -G_e \alpha T \dot{\varepsilon}_{ii} + C_\varepsilon \dot{T} + G_e \varepsilon_{ij} \dot{\varepsilon}_{ij}}$$

Fractional Derivatives

Grünwald-Letnikov definition of the fractional derivative:

$$\frac{\mathrm{d}^{\alpha} f}{\mathrm{d} t^{\alpha}} = \lim_{h \to 0} \frac{1}{h^{\alpha}} \sum_{m=0}^{t/h} (-1)^{m} \frac{\Gamma(\alpha+1)}{m!\,\Gamma(\alpha-m+1)} f(t-mh)$$

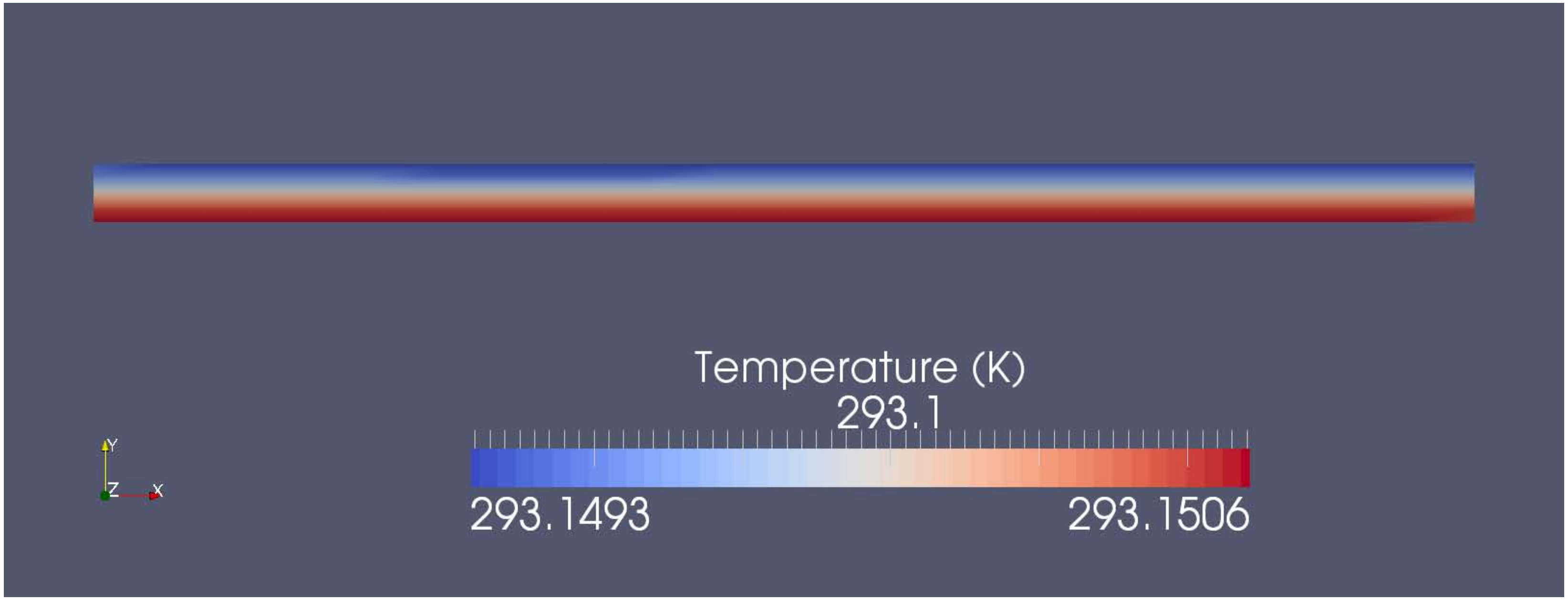
$$\text{where } \Gamma(x) = \int_{0}^{\infty} \exp(-t)\, t^{(x-1)}\, \mathrm{d} t$$

Implementation

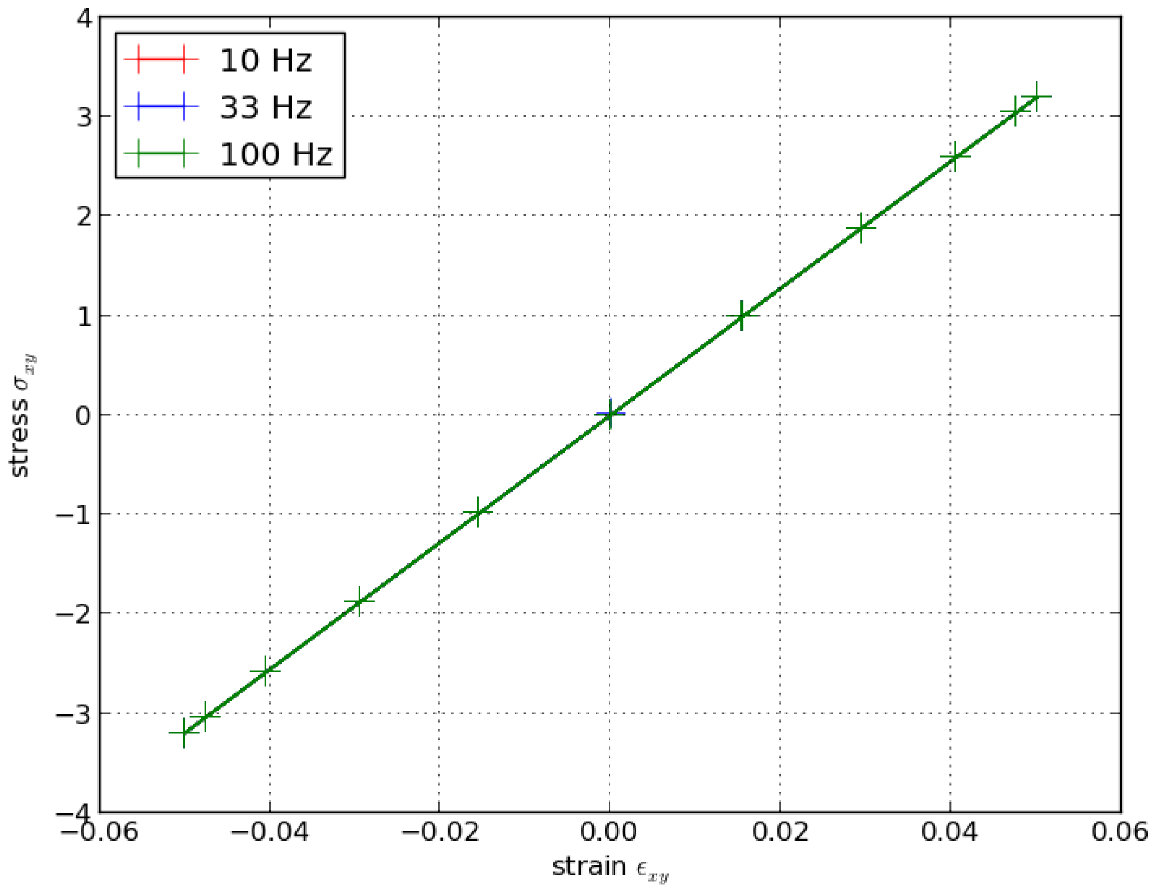
- Solved using FEniCS
  - Also SciPy and NumPy for computations
  - ParaView and matplotlib for plotting the results
- The boundary conditions are:
  - Bottom surface: fixed
  - Top surface: subjected to a oscillating velocity
  - All other surfaces are traction-free
  - Robin boundary condition (convection) for temperature

Results

- Assumed: Properties are not dependent on temperature
- Temperature variation in solution found to be negligible



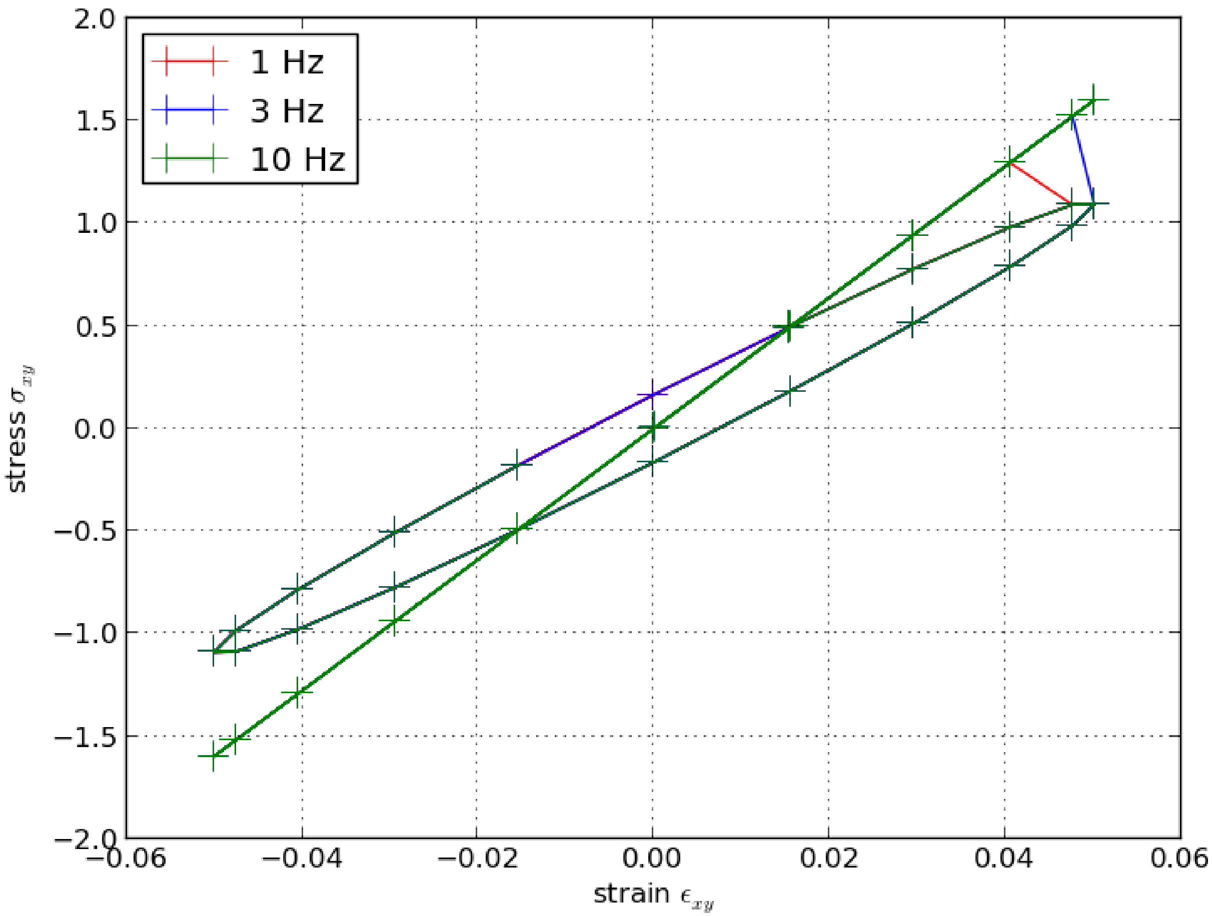
Results



$\tau_0 = 0.0$

$$\sigma_{ij} = G_e \varepsilon_{ij}$$

Results



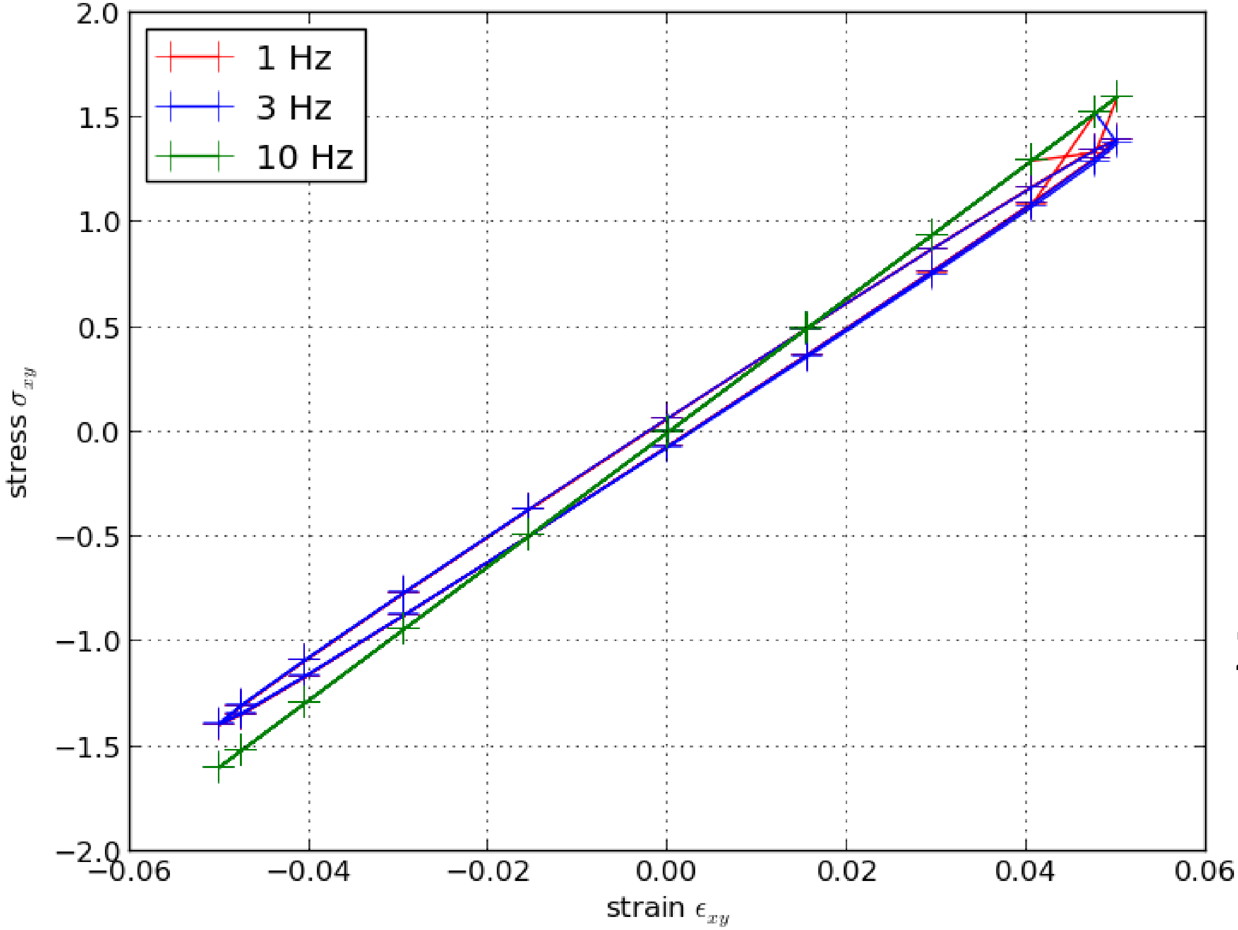
$\alpha = 0$

$\beta = 1$

$\tau_0 = 0.00001$

$$2\sigma_{ij} = 2G_e\varepsilon_{ij} + G_0\tau_0 \frac{\mathrm{d}\,\varepsilon_{ij}}{\mathrm{d}\,t}$$

Results



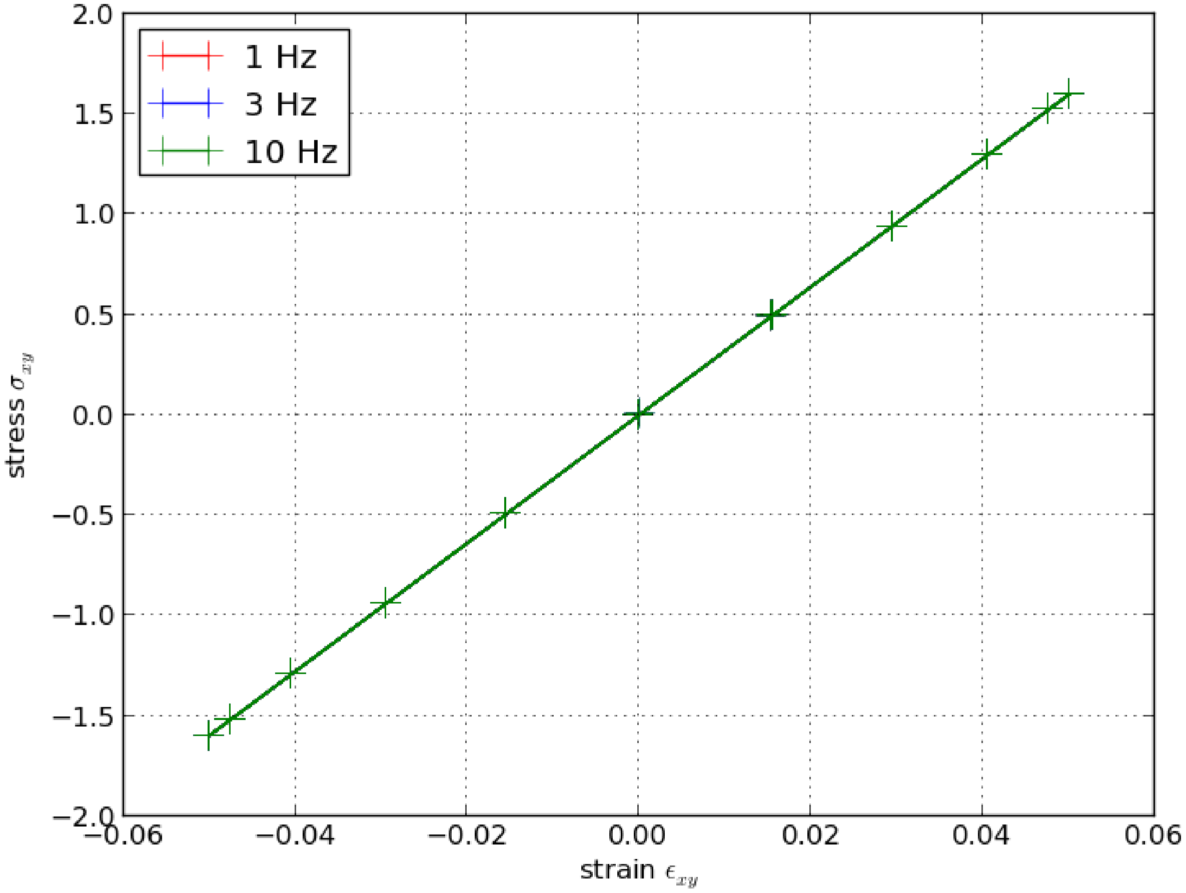
$\alpha = 0$

$\beta = 1.1$

$\tau_0 = 0.00001$

$$2\sigma_{ij} = 2G_e\varepsilon_{ij} + G_0\tau_0^{1.1}\frac{d^{1.1}\varepsilon_{ij}}{dt^{1.1}}$$

Results



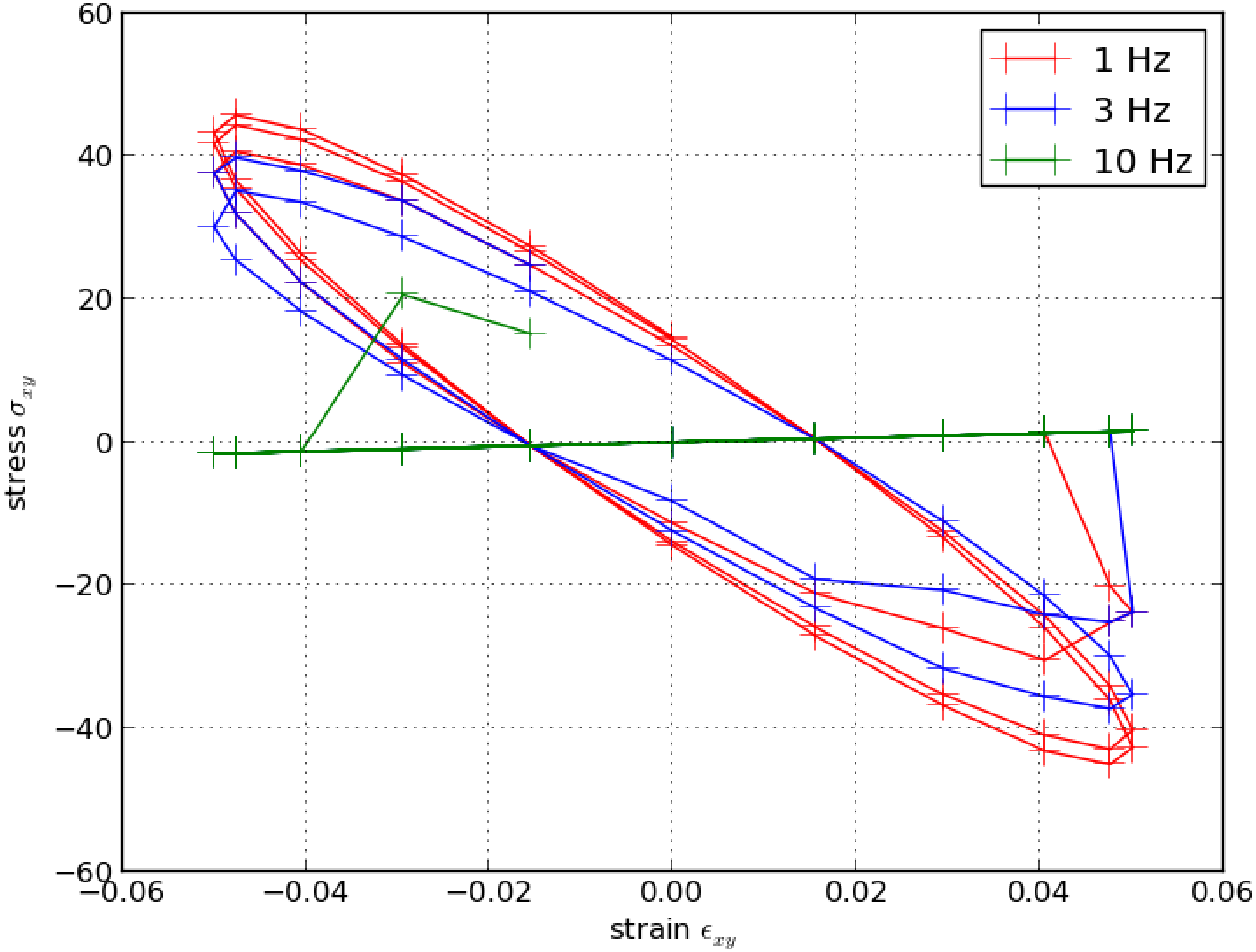
$\alpha = 0$

$\beta = 2$

$\tau_0 = 0.00001$

$$2\sigma_{ij} = 2G_e\varepsilon_{ij} + G_0\tau_0^2 \frac{d^2\,\varepsilon_{ij}}{d\,t^2}$$

Results



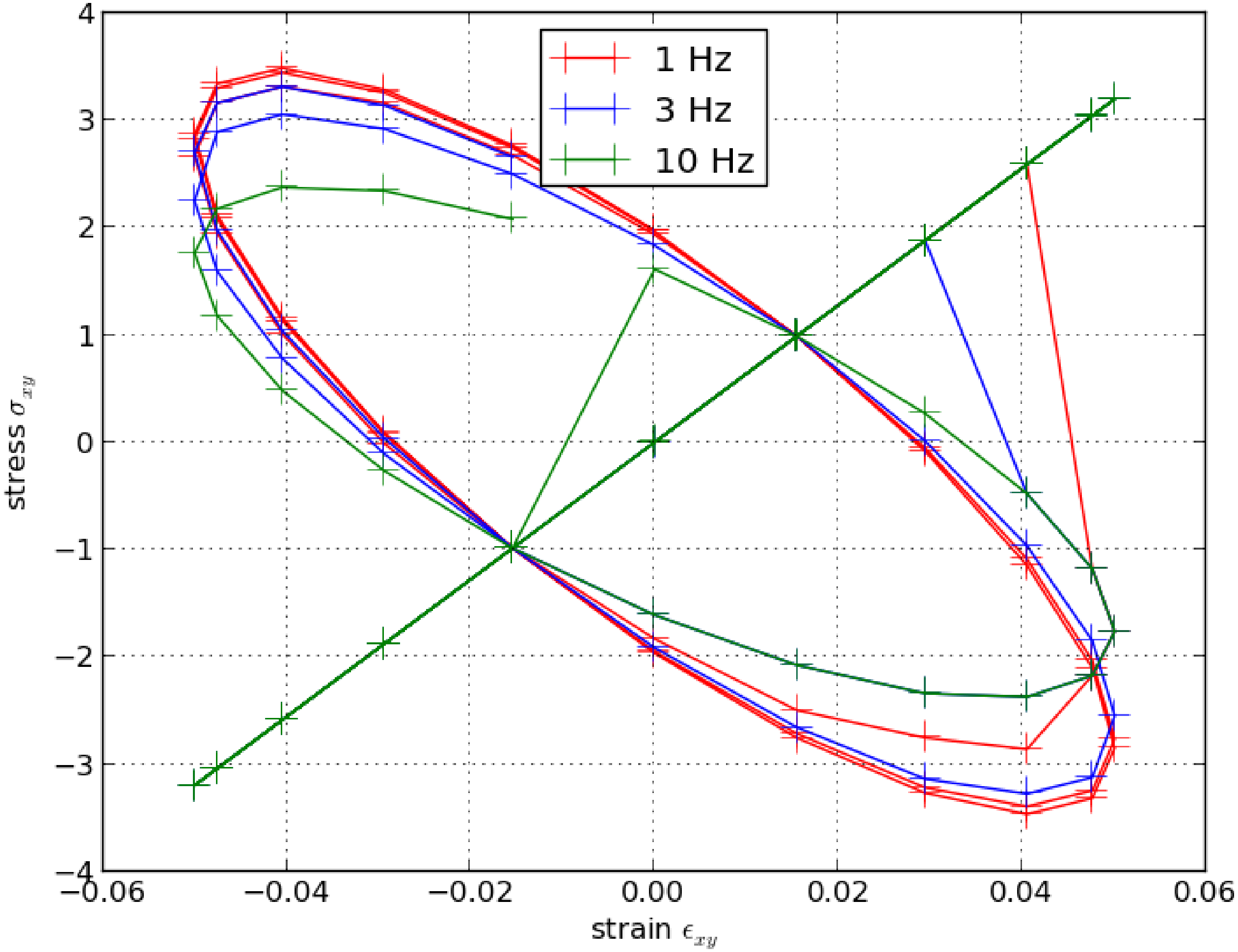
$\alpha = 0$

$\beta = 0.5$

$\tau_0 = 0.00001$

$$2\sigma_{ij} = 2G_e\varepsilon_{ij} + G_0\tau_0^{0.5}\frac{\mathrm{d}^{0.5}\varepsilon_{ij}}{\mathrm{d}t^{0.5}}$$

Results



$\alpha = 0$

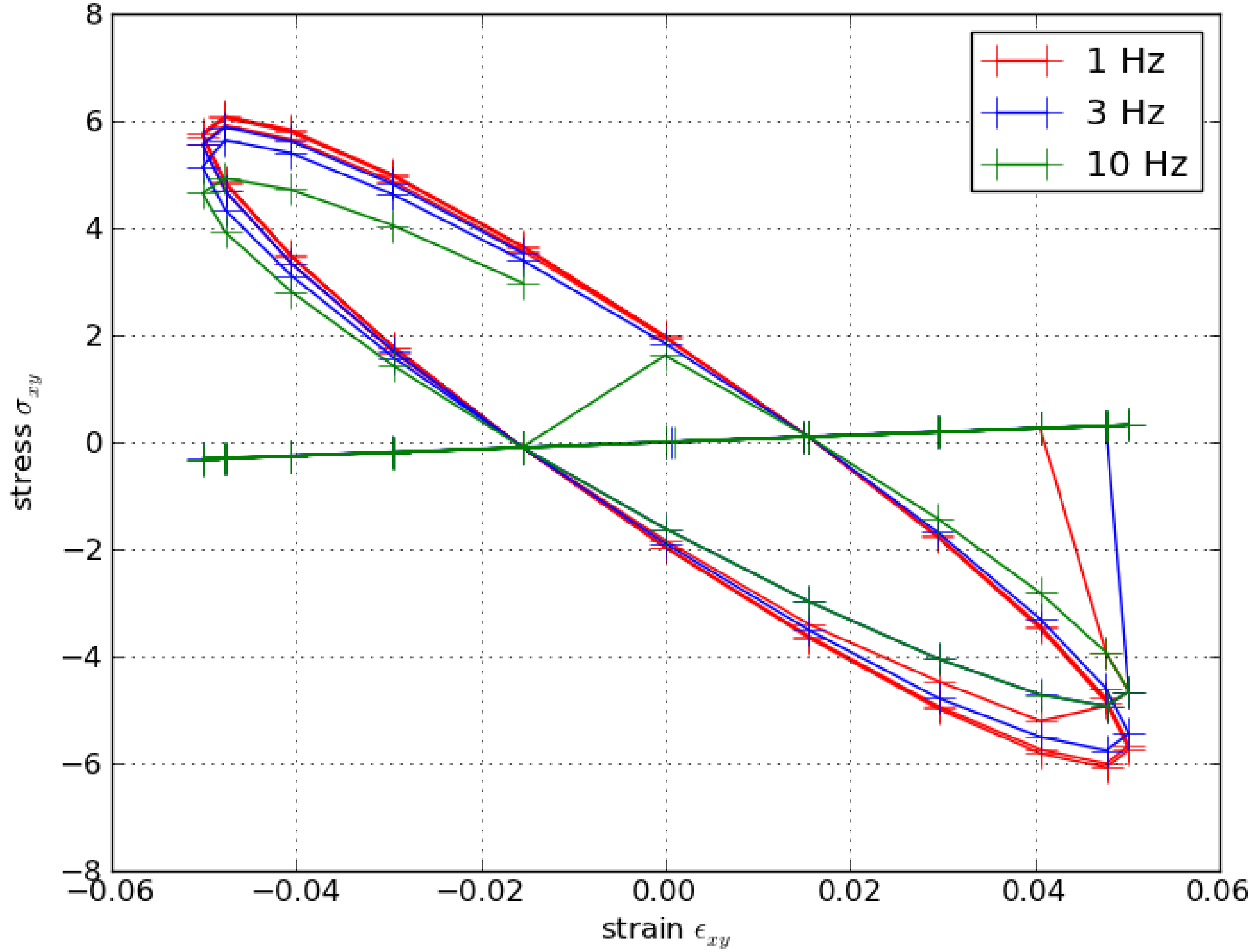
$\beta = 0.5$

$\tau_0 = 0.000001$

$$2\sigma_{ij} = 2G_e\varepsilon_{ij} + G_0\tau_0^{0.5}\frac{\mathrm{d}^{0.5}\varepsilon_{ij}}{\mathrm{d}t^{0.5}}$$

LKM

Results



$\alpha = 0.994$

$\beta = 0.804$

$\tau_0 = 0.00001$

$$\sigma_{ij} + \tau_0^{0.994} \frac{d^{0.994} \sigma_{ij}}{d t^{0.994}}$$

$$= G_e \left(\varepsilon_{ij} + \tau_0^{0.994} \frac{d^{0.994} \varepsilon_{ij}}{d t^{0.994}} \right)$$

$$+ G_0 \tau_0^{0.804} \frac{d^{0.804} \varepsilon_{ij}}{d t^{0.804}}$$

Outlook

- Recoverable stress alone contributes to internal energy?
- Stress negative for strain positive?

LKM

Thanks a lot for your attention!

Questions?