Thermodynamically compatible viscoelastic models suitable for modeling geomaterials

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Asphalt binder

- glue in the asphalt concrete (very sticky)
- almost incompressible (compared to asphalt concrete)
- mixture of a large number of hydrocarbons
- exhibits viscoelastic behavior

Incompressible viscoelastic fluid like models

Balance equations:

$$\operatorname{div} \mathbf{v} = 0,$$

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + [\nabla \mathbf{v}]\mathbf{v} \right) = \operatorname{div} \mathbf{T}, \quad \mathbf{T} = \mathbf{T}^{\mathrm{T}}.$$

Relation for the Cauchy stress tensor $\mathbf{T}$ has to be specified.

$$\mathbf{T} = -p\mathbf{I} + \mathbf{S},$$

rate-type fluid models – $\mathbf{S}$ satisfies *evolutionary* equation.

Standard viscoelastic rate-type fluid models

The Cauchy stress tensor in the form $\mathbf{T} = -p\mathbf{I} + \mathbf{S}$

Maxwell

$$\boxed{\begin{aligned} \mathbf{S} &= G(\mathbf{B} - \mathbf{I}) \\ \overset{\triangledown}{\mathbf{B}} + \frac{1}{\tau}(\mathbf{B} - \mathbf{I}) &= \mathbf{0} \end{aligned}} \qquad \tau = \frac{\mu}{G}$$

Oldroyd-B

$$\boxed{\begin{aligned} \mathbf{S} &= 2\mu_2\mathbf{D} + G(\mathbf{B} - \mathbf{I}) \\ \overset{\triangledown}{\mathbf{B}} + \frac{1}{\tau}(\mathbf{B} - \mathbf{I}) &= \mathbf{0} \end{aligned}} \qquad \tau_1 = \frac{\mu_1}{G}$$

Burgers

$$\boxed{\mathbf{S} + \lambda_1 \overset{\triangledown}{\mathbf{S}} + \lambda_2 \overset{\triangledown\triangledown}{\mathbf{S}} = \eta_1\mathbf{D} + \eta_2 \overset{\triangledown}{\mathbf{D}}}$$

$$\overset{\triangledown}{\mathbf{S}} := \dot{\mathbf{S}} - \mathbf{L}\mathbf{S} - \mathbf{S}\mathbf{L}^{\mathrm{T}}, \quad \mathbf{L} := \nabla\mathbf{v}, \quad \mathbf{D} := \tfrac{1}{2}(\mathbf{L} + \mathbf{L}^{\mathrm{T}})$$

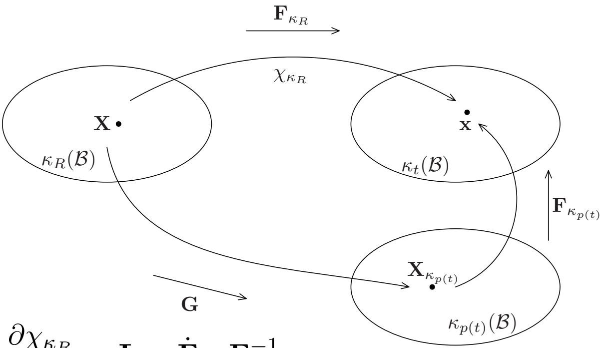
Thermodynamical framework for derivation of viscoelastic models

Experimental data for asphalt binder show interesting phenomena that can not be captured by these standard linear viscoelastic models.

- Rajagopal and Srinivasa (2000), second law of thermodynamics automatically satisfied
- based on the knowledge how the material stores the energy (given by the Helmholtz potential) and how the material dissipates the energy (given by the rate of the entropy production)
- derivation of model by Rajagopal and Srinivasa (2000) was modified and new non-linear model was obtained
- capable of capturing experimental data of viscoelastic fluids
- models reduce to standard Oldroyd-B model

Natural configuration

Using natural configuration the deformation is split into purely elastic and dissipative part.



$$\mathbf{F}_{\kappa_R} = \frac{\partial \chi_{\kappa_R}}{\partial \mathbf{X}}, \quad \mathbf{L} = \dot{\mathbf{F}}_{\kappa_R}\mathbf{F}_{\kappa_R}^{-1}$$

$$\mathbf{B}_{\kappa_{p(t)}} = \mathbf{F}_{\kappa_{p(t)}}\mathbf{F}_{\kappa_{p(t)}}^{\mathrm{T}}, \quad \mathbf{L}_{\kappa_{p(t)}} = \dot{\mathbf{G}}\mathbf{G}^{-1}, \quad \mathbf{D}_{\kappa_{p(t)}} = \frac{\mathbf{L}_{\kappa_{p(t)}} + \mathbf{L}_{\kappa_{p(t)}}^{\mathrm{T}}}{2}$$

$$\dot{\mathbf{B}}_{\kappa_{p(t)}} = \mathbf{L}\mathbf{B}_{\kappa_{p(t)}} + \mathbf{B}_{\kappa_{p(t)}}\mathbf{L}^{\mathrm{T}} - 2\mathbf{F}_{\kappa_{p(t)}}\mathbf{D}_{\kappa_{p(t)}}\mathbf{F}_{\kappa_{p(t)}}^{\mathrm{T}}$$

Two constitutive relations for scalars are prescribed: thermodynamic potential (Helmholtz free energy ψ) and rate of entropy production ξ.

Helmholtz free energy ψ – incompressible neo-Hookean

$$\psi = \frac{G}{2\rho}\left(\operatorname{tr}\mathbf{B}_{\kappa_{p(t)}} - 3\right)$$

Rate of entropy production ξ Rajagopal, Srinivasa (2000) used

$$0 \leq \tilde{\xi} = 2\mu_1 \mathbf{D}_{\kappa_{p(t)}} \cdot \mathbf{B}_{\kappa_{p(t)}} \mathbf{D}_{\kappa_{p(t)}}.$$

We tried several scalars.

Reduced thermodynamic identity; incompressibility conditions

$$\xi = \mathbf{T}\cdot\mathbf{D} - \rho\dot{\psi}; \quad \operatorname{tr}\mathbf{D} = \operatorname{tr}\mathbf{D}_{\kappa_{p(t)}} = 0.$$

Quadratic model with one natural configuration

$$0 \leq \tilde{\xi} = 2\mu_2 \mathbf{D} \cdot \mathbf{D} + 2\mu_1 \mathbf{D}_{\kappa_{p(t)}} \cdot \mathbf{D}_{\kappa_{p(t)}}$$

$$\Downarrow$$

$$\boxed{\begin{aligned} \mathbf{T} &= -p\mathbf{I} + 2\mu_2 \mathbf{D} + G\mathbf{B}^d_{\kappa_{p(t)}}, \\ \overset{\triangledown}{\mathbf{B}}_{\kappa_{p(t)}} &+ \frac{1}{\tau}\mathbf{B}_{\kappa_{p(t)}}\mathbf{B}^d_{\kappa_{p(t)}} = \mathbf{0}. \end{aligned}}$$

$$\mathbf{B}^d_{\kappa_{p(t)}} = \mathbf{B}_{\kappa_{p(t)}} - \frac{1}{3}\left(\operatorname{tr} \mathbf{B}_{\kappa_{p(t)}}\right)\mathbf{I}$$

- it linearizes to standard Oldroyd-B model
- it can be shown that $\det \mathbf{B}_{\kappa_{p(t)}} = 1$ and $\operatorname{tr} \mathbf{B}_{\kappa_{p(t)}} \geq 2$
- it captures one of the experiments

TD compatible Oldroyd-B model

Incompressible total deformation $\det \mathbf{F}_{\kappa_R} = \det \mathbf{G} \det \mathbf{F}_{\kappa_{p(t)}} = 1$
but compressible elastic and dissipative response
$\det \mathbf{G} = 1/\det \mathbf{F}_{\kappa_{p(t)}} \neq 1$

Helmholtz free energy ψ – compressible neo-Hookean

$$\psi = \frac{G}{2\rho}\left(\operatorname{tr}\mathbf{B}_{\kappa_{p(t)}} - 3 - \ln\det\mathbf{B}_{\kappa_{p(t)}}\right)$$

Rate of entropy production ξ

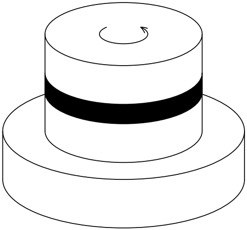
$$0 \leq \tilde{\xi} = 2\mu_2|\mathbf{D}|^2 + 2\mu_1\mathbf{D}_{\kappa_{p(t)}}\mathbf{B}_{\kappa_{p(t)}} \cdot \mathbf{D}_{\kappa_{p(t)}}.$$

Oldroyd-B model

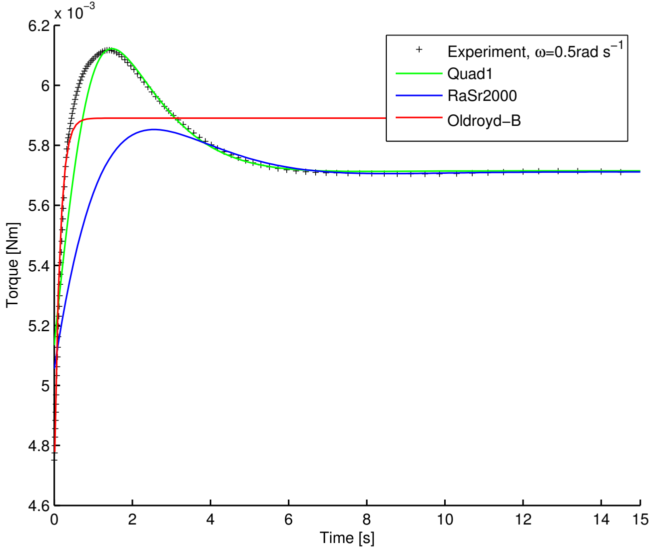
$$\boxed{\begin{gathered}\mathbf{T} = -p\mathbf{I} + 2\mu_2\mathbf{D} + G(\mathbf{B}_{\kappa_{p(t)}} - \mathbf{I}),\\ \overset{\triangledown}{\mathbf{B}}_{\kappa_{p(t)}} + \frac{1}{\tau}(\mathbf{B}_{\kappa_{p(t)}} - \mathbf{I}) = \mathbf{0}.\end{gathered}}$$

Experiment Krishnan, Narayan (2007)

- experiment with asphalt binder
- torsional rheometer, height $h = 1$ mm, radius $R = 4$ mm
- upper plate rotates with constant angular velocity ω
- corresponding torque M is measured



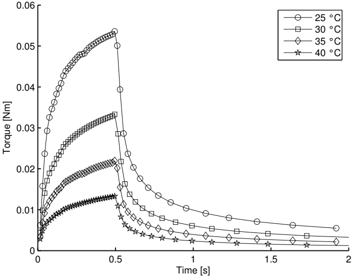
This experiment is fitted in cylindrical coordinates under the assumption that $\mathbf{v} = (0, \omega rz/h, 0)$.

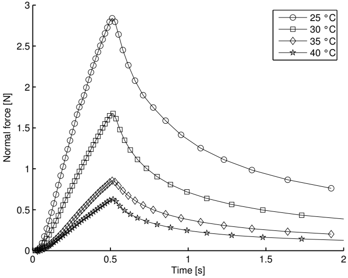


Experiment Narayan et al. (2012)

$$\omega = \begin{cases} 0.5\text{rad s}^{-1} & 0\text{s} \le t \le 0.5\text{s} \\ 0\text{rad s}^{-1} & 0.5\text{s} < t \le 2.0\text{s}. \end{cases}$$

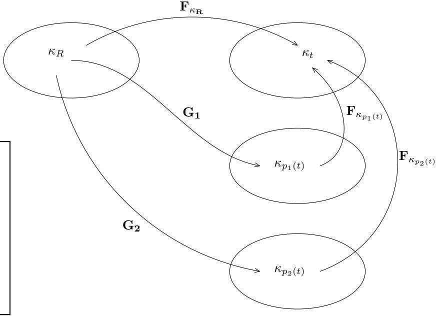
corresponding torque and normal force are measured





Two relaxation mechanisms

Experiments show that ashpalt binders have two different relaxation mechanisms which can be captured by

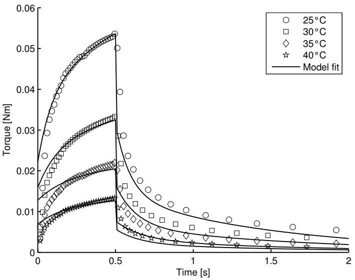


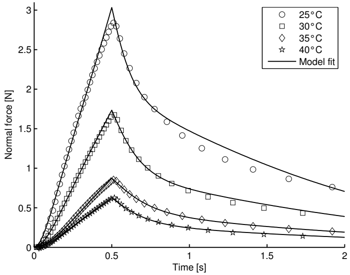
$$\mathbf{T} = -p\mathbf{I} + 2\mu_3\mathbf{D} + G_1\mathbf{B}^d_{\kappa_{p_1(t)}} + G_2\mathbf{B}^d_{\kappa_{p_2(t)}},$$
$$\overset{\triangledown}{\mathbf{B}}_{\kappa_{p_1(t)}} + \frac{1}{\tau_1}\mathbf{B}_{\kappa_{p_1(t)}}\mathbf{B}^d_{\kappa_{p_1(t)}} = \mathbf{0},$$
$$\overset{\triangledown}{\mathbf{B}}_{\kappa_{p_2(t)}} + \frac{1}{\tau_2}\mathbf{B}_{\kappa_{p_2(t)}}\mathbf{B}^d_{\kappa_{p_2(t)}} = \mathbf{0}.$$

reduces to standard Burgers model if the elastic responses are linearized

$$\mathbf{T} = -p\mathbf{I} + 2\mu_3\mathbf{D} + \mathbf{S},$$
$$\mathbf{S} + (\tau_1 + \tau_2)\overset{\triangledown}{\mathbf{S}} + \tau_1\tau_2\overset{\triangledown\triangledown}{\mathbf{S}} = 2(\tau_1 G_1 + \tau_2 G_2)\mathbf{D} + 2\tau_1\tau_2(G_1 + G_2)\overset{\triangledown}{\mathbf{D}}.$$

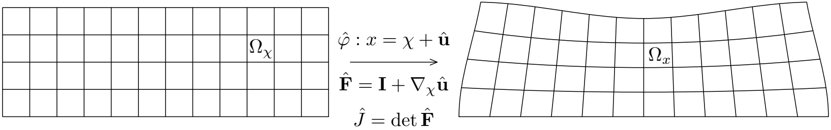
Our fit for experiment Narayan et al. (2012)





Full simulation in deforming domains

- problem computed on a fixed mesh $\Rightarrow$ the weak formulation transformed by $\hat{\varphi}$ from the physical domain in Ω_x to computational domain Ω_χ using arbitrary Langrangian-Eulerian description



- new variable $\hat{\mathbf{u}}$ – arbitrary deformation of the domain and the mesh, for material points the relation $\mathrm{d}\hat{\mathbf{u}}/\mathrm{d}t = \mathbf{v}$ holds
- monolithic approach is used which means that the problem is solved as one big coupled system of equations including the deformation of the mesh

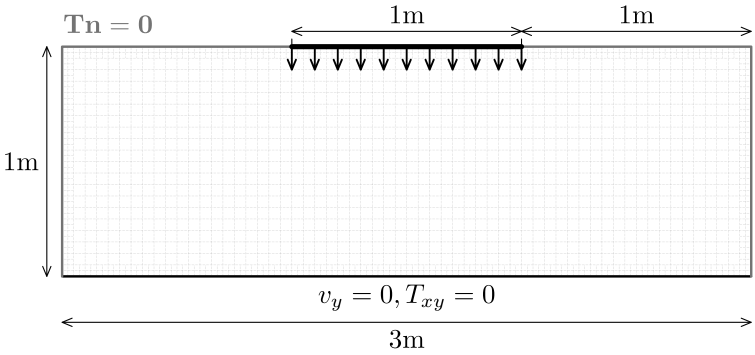
- discretization in time $\frac{\partial y(x,t)}{\partial t} = f\left(y(x,t)\right)$ approximated by conditionally stable ($> 2^{\text{nd}}$ order) Glowinski time scheme

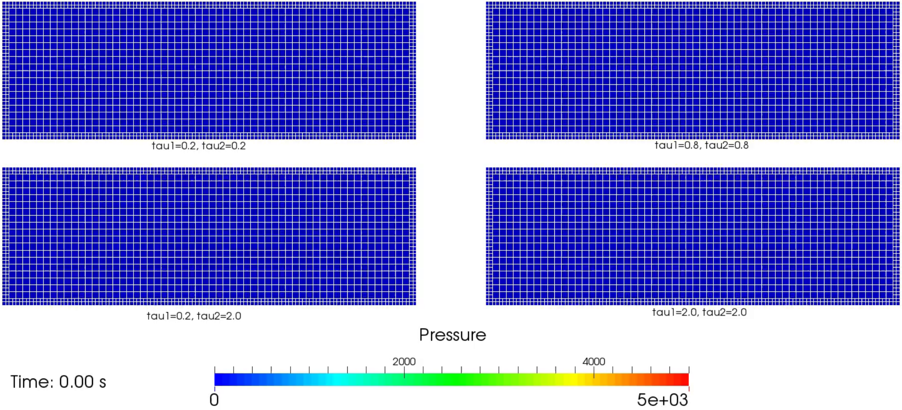
$$
\begin{aligned}
&1. \quad \frac{y^{n+\theta}(x) - y^n(x)}{\theta \Delta t^n} = f\left(y^{n+\theta}(x)\right), \\
&2. \quad y^{n+1-\theta} = \frac{1-\theta}{\theta} y^{n+\theta} + \frac{2\theta - 1}{\theta} y^n, \\
&3. \quad \frac{y^{n+1}(x) - y^{n+1-\theta}(x)}{\theta \Delta t^n} = f\left(y^{n+1}(x)\right).
\end{aligned}
$$

- discretization in space, quadrilaterals, refined near boundary
- pressure p / velocity $\mathbf{v}$ / deformation $\mathbf{u}$ / tensor $\mathbf{B}_{\kappa_{p(t)}}$ approximated by $\mathsf{P}_1^{\text{disc}}$ / Q_2 / Q_2 / Q_2
- Newton method & UMFPACK
- based on J. Hron's code, tests with benchmarks

Pressing of viscoelastic material

- rectangular piece of material, width 3m, height 1m
- material is on the ground: it can fully slip in the x-direction, but it can not flow in the y-direction
- all other sides of the rectangle are free
- at $t = 0$ the material is at rest, and it is suddenly pushed in the middle at the top with a constant normal stress $Tyy =$ -5 kPa for $\Delta t = 0.5$ s




tau1=0.2, tau2=0.2
tau1=0.8, tau2=0.8
tau1=0.2, tau2=2.0
tau1=2.0, tau2=2.0
Pressure
Time: 0.00 s
2000
4000
0
5e+03

Experimental order of convergence

- problem computed with Oldroyd-B model and $\tau = 0.8$ s
- using four different mesh sizes h and four different time steps Δt
- compared $E_k(h, \Delta t)$ and $u_y(h, \Delta t)$ in the middle of the top side at $t = 0.6$ s
- experimental order of convergence estimated by fitting both solutions E_k and u_y by

$$a_0 + a_1 h^{b_1} + a_2 \Delta t^{b_2}$$

and obtained

$$u_y = -0.10463466 - 0.0368\ h^{1.108} - 3.6160\ \Delta t^{2.812}$$
$$E_k = 92.075101 + 44.735\ h^{0.997} + 313.522\ \Delta t^{1.876}$$

values to which the solutions converge and experimental order of convergence.

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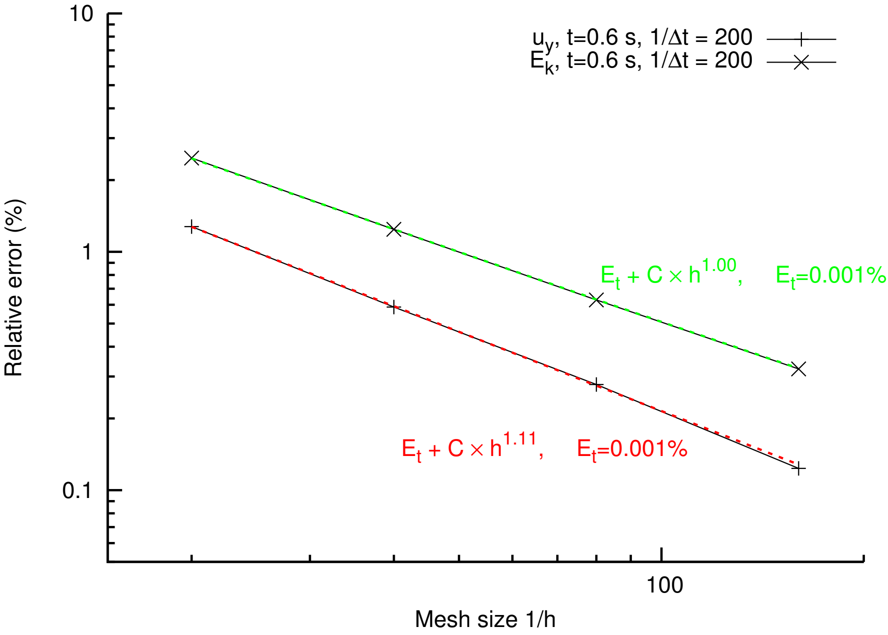
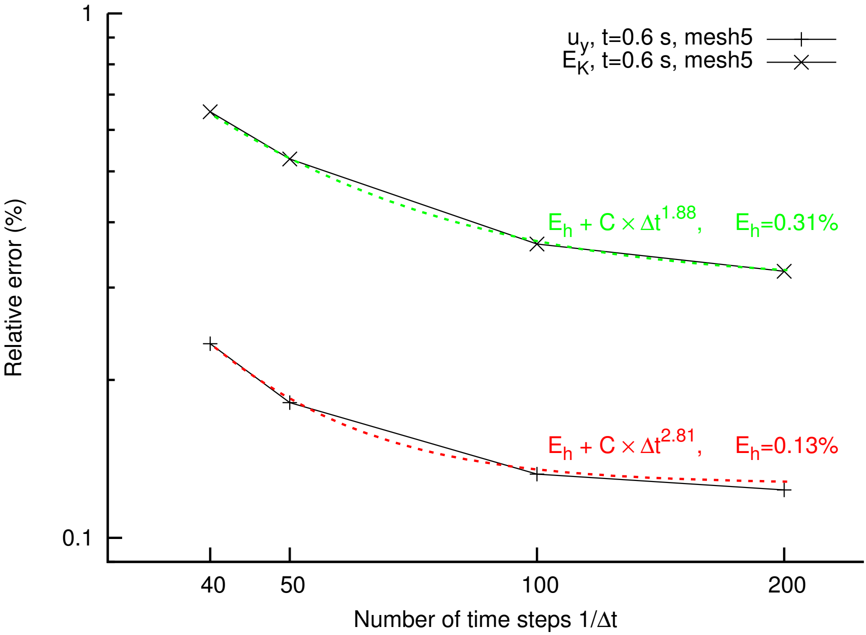
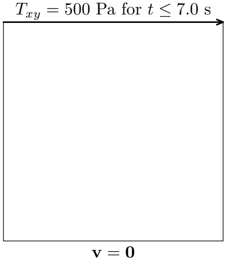


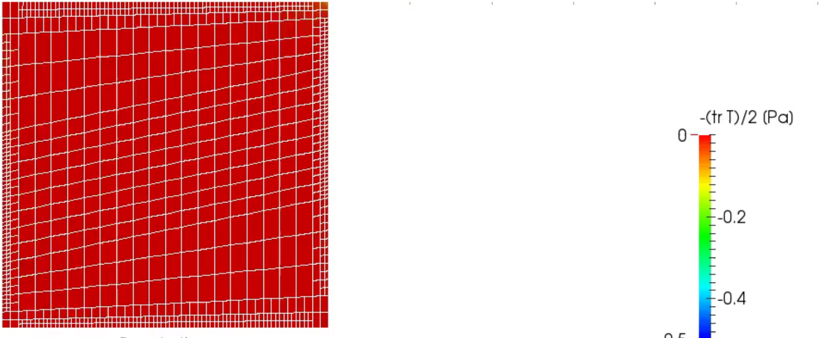
10
1
0.1
100
Relative error (%)
Mesh size 1/h
u_y, t=0.6 s, 1/Δt = 200
E_k, t=0.6 s, 1/Δt = 200
E_t + C × h^1.00, E_t=0.001%
E_t + C × h^1.11, E_t=0.001%


1
0.1
Relative error (%)
40
50
100
200
Number of time steps 1/Δt
u_y, t=0.6 s, mesh5
E_K, t=0.6 s, mesh5
E_h + C × Δt^1.88, E_h=0.31%
E_h + C × Δt^2.81, E_h=0.13%

Applying shear stress on a square from the viscoelastic material

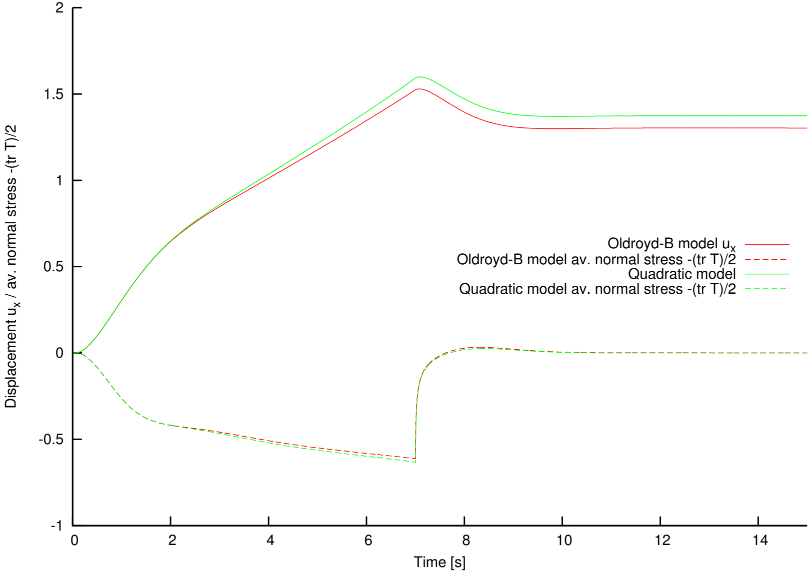
- square piece of material, side 1m
- bottom side fixed, other sides free
- apply shear stress $T_{xy} = 500$ Pa on the top side for $0 \leq t \leq 7.0$
- $\rho = 1000$ kg m^{-3}, $\mu_2 = 1$ kPa s, $G = 1$ kPa, $\tau = 2.0$ s
- computed for Oldroyd-B and quadratic model





Quadratic

Dependence of u_x and $-(\mathrm{tr}\,\mathbf{T})/2$ w.r.t t



Summary of the results

- models equivalent to standard Maxwell, Oldroyd-B or Burgers:
  - can be obtained using thermodynamic approach
  - satisfy the second law of themodynamics
  - one should view them as the fluids where the elastic response corresponds to that of a compressible neo-Hookean solid
- however they do not agree with the experiments – new TD compatible non-linear models that capture the experiments were derived
- computation in time varying domain using ALE method – real life problems