Viscoelasticity in mantle convection

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Content

I2ELVIS - Taras Gerya

- staggered grid, markers
- regional studies, benchmarks
- 3D version not elastic yet - I3VIS

Ellipsis - Moresi, Muhlhaus

- finite elements, markers used as integration points
- regional studies

StagYY - Paul Tackley

- staggered grid, global studies, 3D, spherical shell
- not elastic yet

Extended Boussinesq - nondimensionalised

equation of motion + continuity + thermal equation

$$-\nabla p + \nabla \cdot \sigma = -\mathrm{Ra}\, T\, \vec{e}_z$$

$$\nabla \cdot \vec{v} = 0$$

$$\frac{\partial T}{\partial t} = \nabla^2 T - \vec{v} \cdot \nabla T$$

rheology

$$\sigma + \mathcal{D} \overset{\triangledown}{\sigma} = 2\eta \mathbb{D}$$

$$\eta(p, T) = \exp(-\mathrm{A}(T - T_{ref}) + \mathrm{B}(p - p_{ref}))$$

Constitutive equation

$$\sigma + \mathcal{D}\overset{\nabla}{\sigma} = 2\eta\mathbb{D} \qquad \mathcal{D}(p,T) := \tau_{\mathrm{rel}}\frac{\kappa}{h^2} = \frac{\eta\kappa}{Gh^2}$$

$$\overset{\nabla}{\sigma} := \frac{\partial\sigma}{\partial t} + (\vec{v}\nabla)\,\sigma + (\sigma\mathbb{W} - \mathbb{W}\sigma) - \mathrm{a}(\mathbb{D}\sigma + \sigma\mathbb{D})$$

advection co-rotation co-deformation

Discretization (mixed euler, 1st order accurate)

$$\sigma^n = \frac{\mathrm{d}t}{\mathrm{d}t + \mathcal{D}}2\eta\mathbb{D}^n + \frac{\mathcal{D}}{\mathrm{d}t + \mathcal{D}}\sigma^{n-1} + \frac{\mathcal{D}\,\mathrm{d}t}{\mathrm{d}t + \mathcal{D}}(\mathbb{W}\sigma - \sigma\mathbb{W} + \mathrm{a}(\mathbb{D}\sigma + \sigma\mathbb{D}))$$

$$\sigma^n = \frac{\mathrm{d}t}{\mathrm{d}t + \mathcal{D}} 2\eta \mathbb{D}^n + \frac{\mathcal{D}}{\mathrm{d}t + \mathcal{D}} \left(\sigma^{n-1} + \mathrm{d}t \left(\mathbb{W}\sigma - \sigma\mathbb{W} + \mathrm{a} \left(\mathbb{D}\sigma + \sigma\mathbb{D} \right) \right) \right)$$

$$\tilde{\sigma}^{n-1} := \sigma^{n-1} + \mathrm{d}t \left(\mathbb{W}\sigma - \sigma\mathbb{W} + \mathrm{a} \left(\mathbb{D}\sigma + \sigma\mathbb{D} \right) \right)^{n-1/n}$$

$$\sigma^n = 2\eta^n_{\mathrm{num}} \mathbb{D}^n + \frac{\mathcal{D}^n}{\mathrm{d}t + \mathcal{D}^n} \tilde{\sigma}^{n-1}; \qquad \eta_{\mathrm{num}} := \frac{\mathrm{d}t}{\mathrm{d}t + \mathcal{D}} \eta$$

Viscoelasticity parameter Z

$$\mathrm{Z} := \frac{\mathrm{d}t}{\mathrm{d}t + \mathcal{D}}; \qquad \sigma^{\mathrm{n}} = 2\,\mathrm{Z}\,\eta^{\mathrm{n}}\,\mathbb{D}^{\mathrm{n}} + (1 - \mathrm{Z})\,\tilde{\sigma}^{\mathrm{n}-1}$$

$$\mathrm{d}t^{\mathrm{n-1,n}} = \text{stability}(\vec{v}^{\mathrm{n-1}}, \mathcal{D}, d); \quad \mathrm{d}t^{\mathrm{a}}; \quad \mathrm{d}t^{\mathrm{el}}$$

$$T^{\mathrm{n}} = \text{advection-diffusion}\,(T^{\mathrm{n-1}}, \vec{v}^{\mathrm{n-1}}, \mathrm{d}t^{\mathrm{a}})$$

$$\tilde{\sigma}^{\mathrm{n-1}} = \sigma^{\mathrm{n-1}} + \text{deadvection}\,(\sigma^{\mathrm{n-1}}, \vec{v}^{\mathrm{n-1}}, \mathrm{d}t^{\mathrm{a}})$$

$$\eta^{\mathrm{n}} = \eta(T^{\mathrm{n}}); \qquad \eta^{\mathrm{n}}_{\mathrm{num}} = \eta^{\mathrm{n}}_{\mathrm{num}}(\eta^{\mathrm{n}}, \mathrm{d}t^{\mathrm{el}}, \mathcal{D}^{\mathrm{n}})$$

$$\text{rhs}^{\mathrm{n}} = \nabla \cdot \left(\frac{\mathcal{D}^n}{\mathrm{d}t^{\mathrm{el}} + \mathcal{D}^n}\, \tilde{\sigma}^{n-1} \right) - \mathrm{Ra}\, T^{\mathrm{n}}\, \vec{e}_z$$

$$\text{Stokes}(\eta^{\mathrm{n}}_{\mathrm{num}}, \vec{v}^{\mathrm{n}}, p^{\mathrm{n}}) = \text{rhs}^{\mathrm{n}}$$

$$\sigma^n = \sigma^n(\tilde{\sigma}^{n-1}, \eta^{\mathrm{n}}_{\mathrm{num}}, \vec{v}^{\mathrm{n}})$$

no decoupling:

$$\mathrm{d}t^{\mathrm{a}} = \mathrm{d}t^{\mathrm{n-1,n}}$$

$$\mathrm{d}t^{\mathrm{el}} = \mathrm{d}t^{\mathrm{n-1,n}}$$

Harder - *Journal of Non-Newtonian Fluid Mechanics*, 39 (1991) 67-88

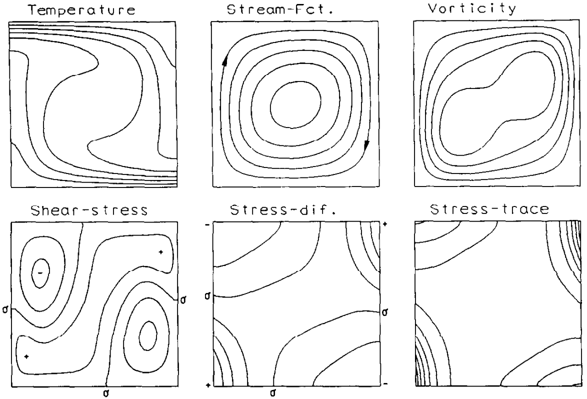
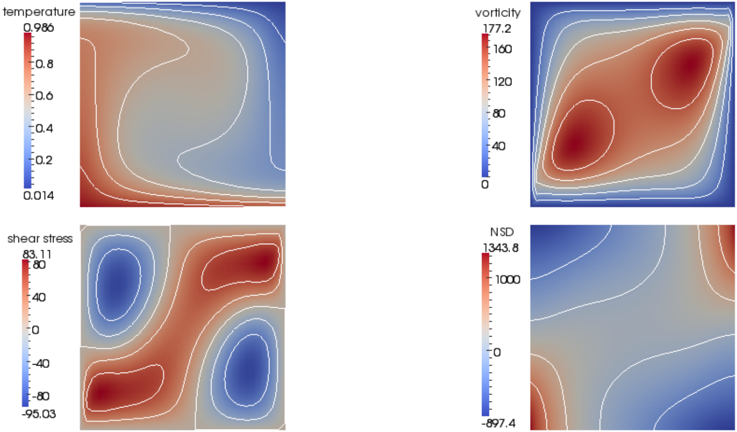
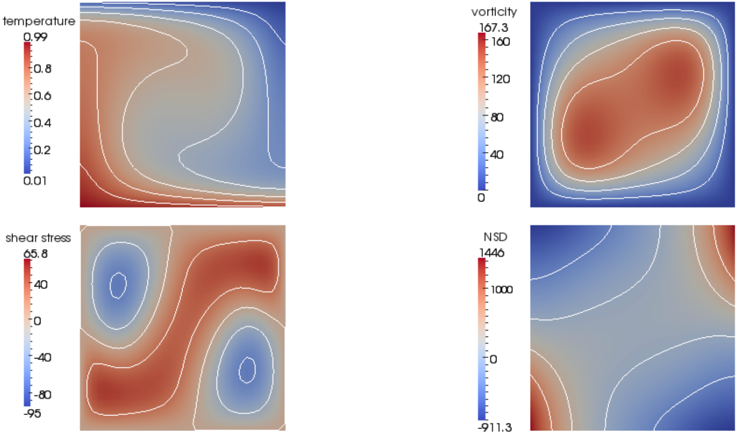


Fig. 5. As Fig. 4, but with upper convected Maxwell rheology ($a = 1$, $\lambda = 0.0015$, $De = 0.34$). Additional isolines for the stress trace: $\mu(75, 275, \ldots, 1075)$.

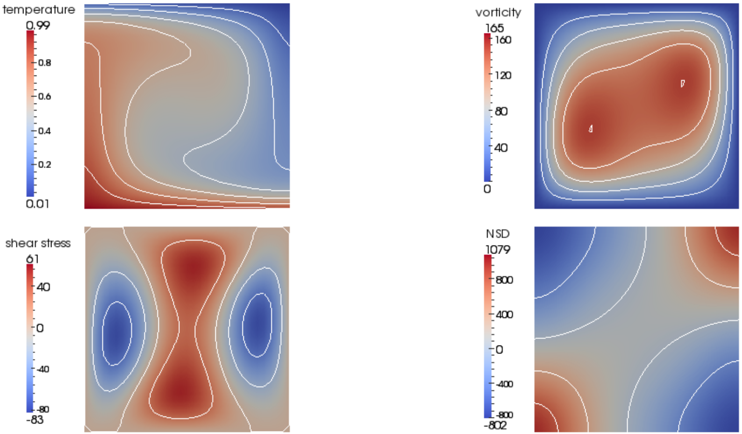
Co-rotational derivative (Jaumann, $a = 0$)



Upper convected derivative $(a = 1)$

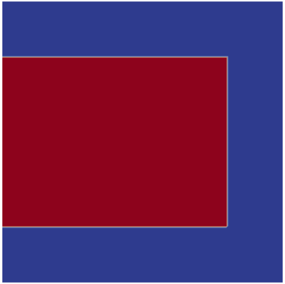


Viscous case



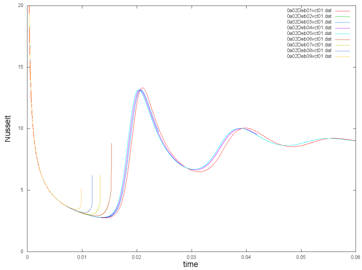
Bending of an elastic slab (under gravity for 20 Kyr)

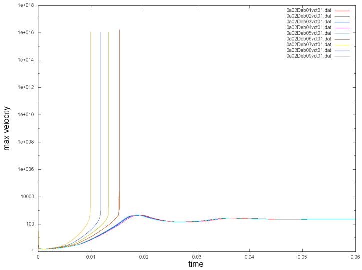
$$\rho_1 = 4000; \quad \eta_1 = 1\,\mathrm{e}27; \quad G_1 = 1\,\mathrm{e}10;$$
$$\rho_2 = 1; \quad \eta_2 = 1\,\mathrm{e}21; \quad G_2 = 1\,\mathrm{e}20;$$



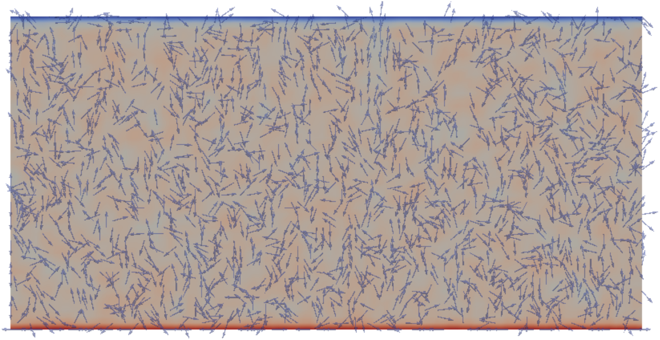
Onset of convection is related to "numerically instaneous" elastic behaviour for Deborah number above certain critical value.

$$\mathrm{Ra} = 10^4 \rightarrow \mathcal{D}_{critical} = 1.5 \cdot 10^{-3}$$

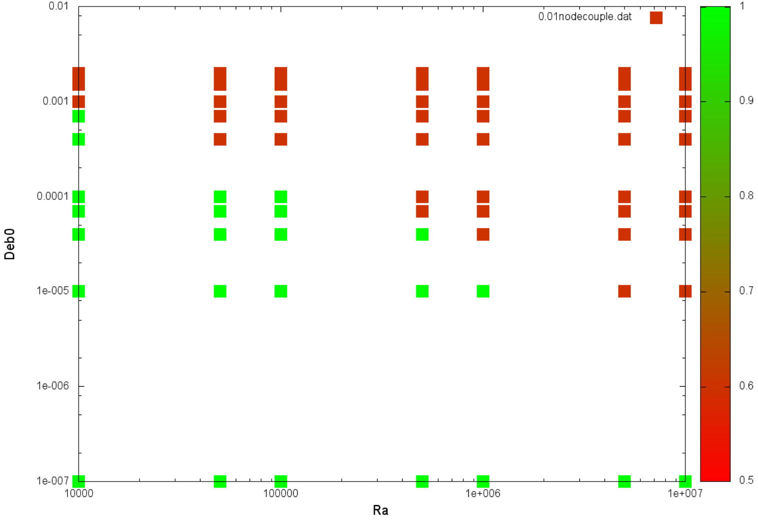




Example of velocity singularity



Jaumann - parametric study, failed runs



$$\mathrm{d}t^{\mathrm{n-1,n}} = \text{stability}(\vec{v}^{\mathrm{n-1}}, \mathcal{D}, d); \quad \mathrm{d}t^{\mathrm{a}}; \quad \mathrm{d}t^{\mathrm{el}}$$

$$T^{\mathrm{n}} = \text{advection-diffusion}\,(T^{\mathrm{n-1}}, \vec{v}^{\mathrm{n-1}}, \mathrm{d}t^{\mathrm{a}})$$

$$\tilde{\sigma}^{\mathrm{n-1}} = \sigma^{\mathrm{n-1}} + \text{deadvection}\,(\sigma^{\mathrm{n-1}}, \vec{v}^{\mathrm{n-1}}, \mathrm{d}t^{\mathrm{a}})$$

$$\eta^{\mathrm{n}} = \eta(T^{\mathrm{n}}); \qquad \eta^{\mathrm{n}}_{\mathrm{num}} = \eta^{\mathrm{n}}_{\mathrm{num}}(\eta^{\mathrm{n}}, \mathrm{d}t^{\mathrm{el}}, \mathcal{D}^{\mathrm{n}})$$

$$\text{rhs}^{\mathrm{n}} = \nabla \cdot \left(\frac{\mathcal{D}^n}{\mathrm{d}t^{\mathrm{el}} + \mathcal{D}^n} \tilde{\sigma}^{n-1} \right) - \mathrm{Ra}\, T^{\mathrm{n}} \vec{e}_z$$

$$\text{Stokes}(\eta^{\mathrm{n}}_{\mathrm{num}}, \vec{v}^{\mathrm{n}}, p^{\mathrm{n}}) = \text{rhs}^{\mathrm{n}}$$

$$\sigma^n = \sigma^n(\tilde{\sigma}^{n-1}, \eta^{\mathrm{n}}_{\mathrm{num}}, \vec{v}^{\mathrm{n}})$$

Gerya / Moresi decoupling: multiple advection

Time step decoupling

$$\mathrm{d}t^{\mathrm{n-1,n}} = \text{stability}(\vec{v}^{\mathrm{n-1}}, \mathcal{D}, d); \quad \mathrm{d}t^{\mathrm{a}}; \quad \mathrm{d}t^{\mathrm{el}}$$

$$T^{\mathrm{n}} = \text{advection-diffusion}\,(T^{\mathrm{n-1}}, \vec{v}^{\mathrm{n-1}}, \mathrm{d}t^{\mathrm{a}})$$

$$\tilde{\sigma}^{\mathrm{n-1}} = \sigma^{\mathrm{n-1}} + \text{deadvection}\,(\sigma^{\mathrm{n-1}}, \vec{v}^{\mathrm{n-1}}, \mathrm{d}t^{\mathrm{a}})$$

$$\eta^{\mathrm{n}} = \eta(T^{\mathrm{n}}); \qquad \eta^{\mathrm{n}}_{\mathrm{num}} = \eta^{\mathrm{n}}_{\mathrm{num}}(\eta^{\mathrm{n}}, \mathrm{d}t^{\mathrm{el}}, \mathcal{D}^{\mathrm{n}})$$

$$\text{rhs}^{\mathrm{n}} = \nabla \cdot \left(\frac{\mathcal{D}^n}{\mathrm{d}t^{\mathrm{el}} + \mathcal{D}^n} \tilde{\sigma}^{n-1} \right) - \mathrm{Ra}\, T^{\mathrm{n}}\, \vec{e}_z$$

$$\text{Stokes}(\eta^{\mathrm{n}}_{\mathrm{num}}, \vec{v}^{\mathrm{n}}, p^{\mathrm{n}}) = \text{rhs}^{\mathrm{n}}$$

$$\sigma^n = \sigma^n(\tilde{\sigma}^{n-1}, \eta^{\mathrm{n}}_{\mathrm{num}}, \vec{v}^{\mathrm{n}})$$

convection decoupling:

interpolation needed

Realistic case: separate viscous and viscoelastic parts of the domain

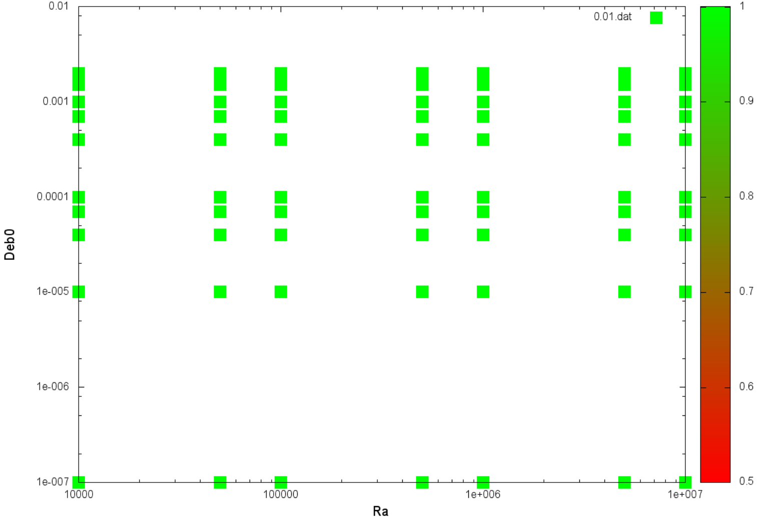
$$\mathrm{Z} := \frac{\mathrm{d}t^{\mathrm{el}}}{\mathrm{d}t^{\mathrm{el}} + \mathcal{D}}; \qquad \sigma^{\mathrm{n}} = 2\,\mathrm{Z}\,\eta^{\mathrm{n}}\,\mathbb{D}^{\mathrm{n}} + (1-\mathrm{Z})\,\tilde{\sigma}^{\mathrm{n}-1}$$

bulid-up relaxation

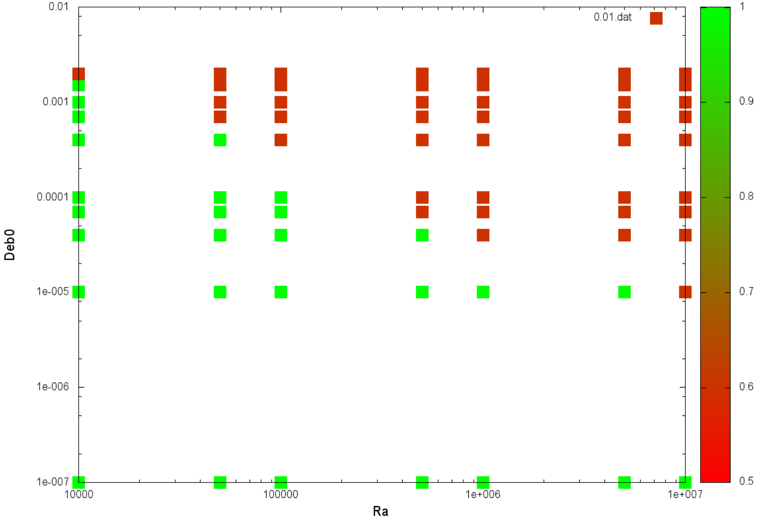
Desired behaviour: viscoelastic material does not move across many cells within elastic time step (viscous material can - elastic time step does not play any role in viscous part of the domain).

$$\mathcal{D} = \eta\mathcal{D}_0; \qquad \mathrm{d}t^{\mathrm{el}} = 0.01\,\tau_{\mathrm{rel}}\frac{\kappa}{h^2} = 0.01\,\mathcal{D}_0; \qquad \mathrm{Z} = \frac{1}{1+\frac{\eta}{0.01}};$$

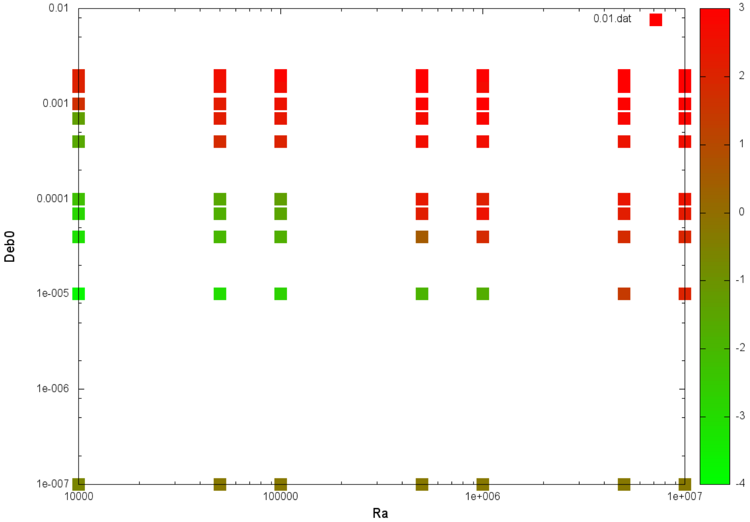
Jaumann - failed runs, decoupled



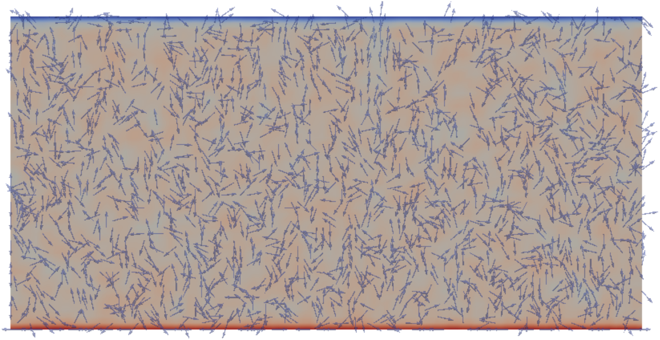
Upper convected - failed runs, decoupled



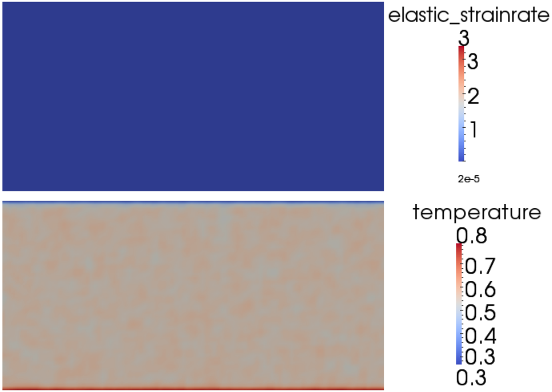
Jaumann - not "trusted" runs, decoupled



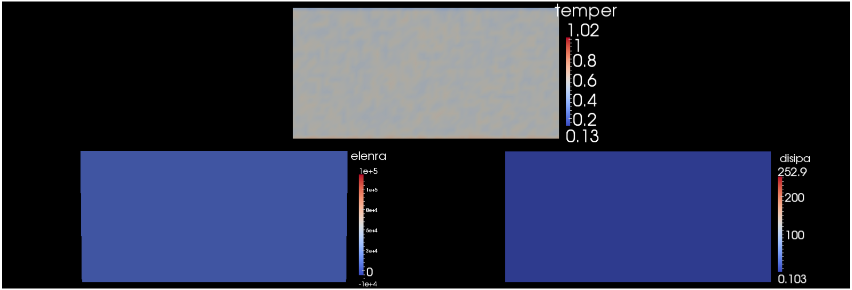
Critical Deborah, time step decoupled



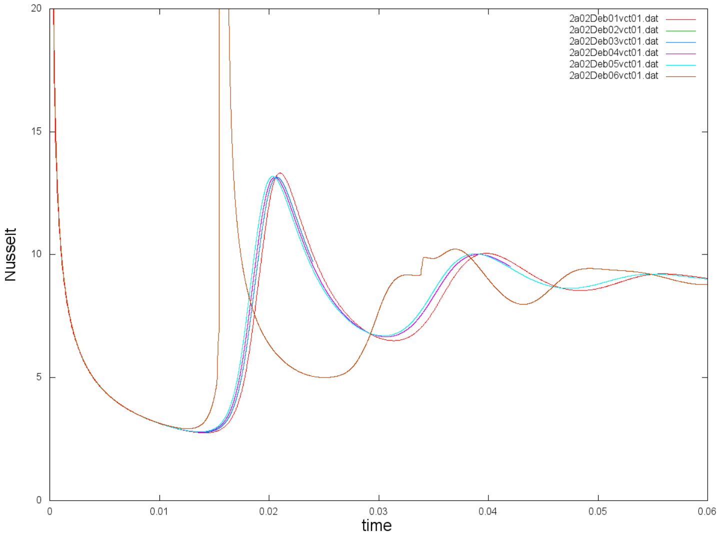
Critical Deborah, time step decoupled: elastic strain rate



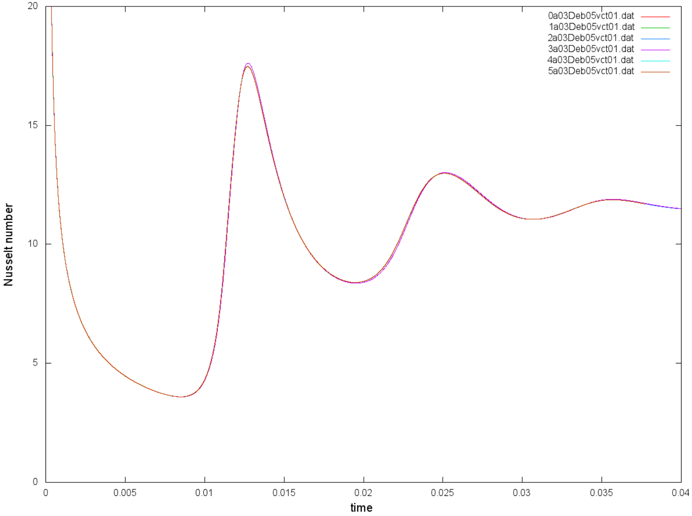
Critical Deborah, time step decoupled: upper convected



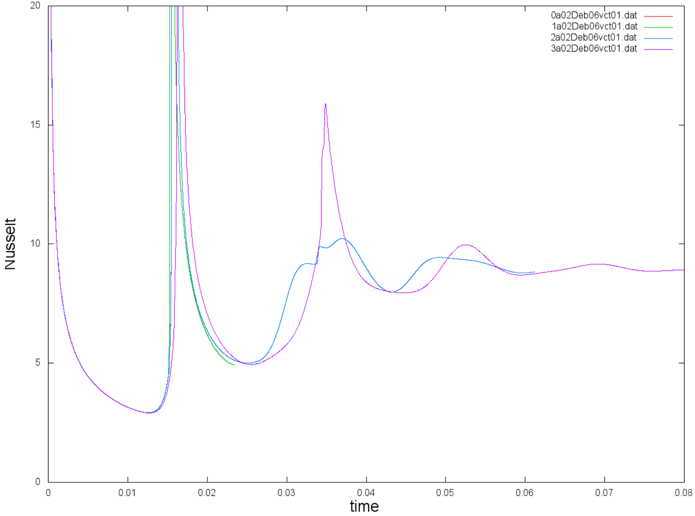
Elastic episodes



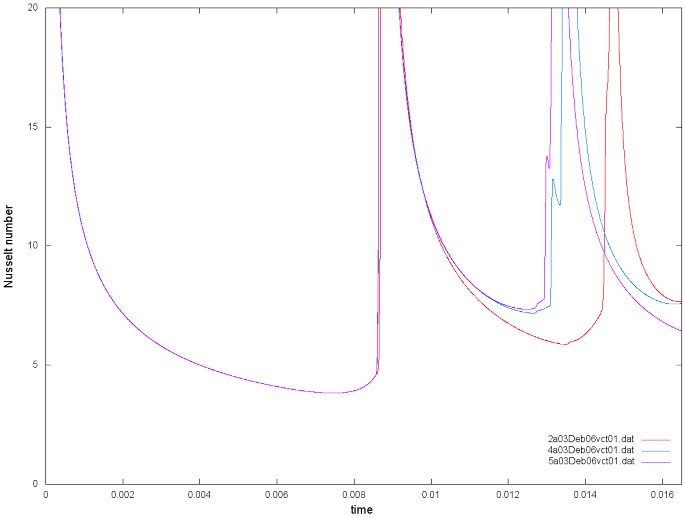
Undercritical Deborah number - time step/scheme convergence



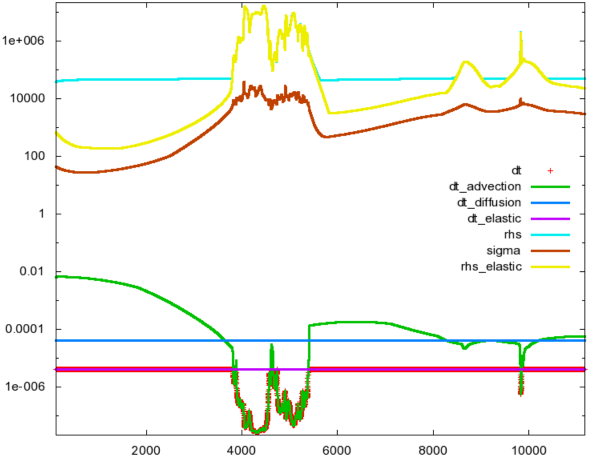
Overcritical Deborah number - time step convergence



Overcritical Deborah number - time scheme convergence



Time step analysis - overcritical Deborah number



Four ways to derive our rheological equation

- 1D analogs
  - objective rate not specified
- Entropy production maximization
  - dissipation needs to be prescribed
  - objective rate specified
- 3D analogs - is it new?
  - objective rate specified
- Microscopical model
  - e.g. dumbbells diluted in newtonian fluid

We need to know how the equation was derived for interpretation: elastic strain rate, elastic energy, dissipation ...

3D analogs

Geodynamical texts often use $\sigma_{ij} = 2\eta\dot{\varepsilon}_{ij}$ - incorrect

Four possible strain tensors: eulerian/lagrangian, full/linearized

$$\varepsilon^{\mathrm{lin}} := \frac{1}{2}\left(\nabla u + (\nabla u)^{\mathrm{T}}\right); \qquad \xi^{\mathrm{lin}} := \frac{1}{2}\left(\mathrm{Grad}\, U + (\mathrm{Grad}\, U)^{\mathrm{T}}\right)$$

$$\varepsilon := \frac{1}{2}(\mathbb{I} - \mathbb{F}^{-\mathrm{T}}\mathbb{F}^{-1}); \qquad \xi := \frac{1}{2}\left(\mathbb{F}^{\mathrm{T}}\mathbb{F} - \mathbb{I}\right)$$

which have following material time derivatives

$$\dot{\varepsilon}^{\mathrm{lin}} = \mathbb{D} - \frac{1}{2}((\nabla u)\mathbb{L} + \mathbb{L}^{\mathrm{T}}(\nabla u)^{\mathrm{T}}) \qquad \dot{\varepsilon} = \mathbb{D} - (\varepsilon\mathbb{L} + \mathbb{L}^{\mathrm{T}}\varepsilon)$$

$$\dot{\xi}^{\mathrm{lin}} = \mathbb{D} - \frac{1}{2}((\nabla u)^{\mathrm{T}}\mathbb{L}^{\mathrm{T}} + \mathbb{L}(\nabla u)) \qquad \dot{\xi} = \mathbb{F}^{\mathrm{T}}\,\mathbb{D}\,\mathbb{F}$$

Maxwell rheology is based on this idea:

Elastic and viscous deformations add together, but stress is the same for both elastic and viscous parts of the deformation

$$\tau = -p + \sigma; \quad \mathbb{D} = \mathbb{D}^{\text{vis}} + \mathbb{D}^{\text{el}}$$

$$\sigma = 2\eta\mathbb{D}^{\text{vis}} = 2G\varepsilon^{\text{el}}$$

Choice of ε or ξ or ε^{lin} or ξ^{lin} gives us the relation $\varepsilon^{\text{el}} \to \mathbb{D}^{\text{el}}$ and thus specifies the rate used in our rheology (only for ε we get an objective rate - lower convected one)

Entropy production maximization

Motivation - interpretation of physical quantities:
what is dissipation, elastic strain rate, elastic energy ...

$$\sigma : \nabla \vec{v} = \sigma : \mathbb{D} = \frac{\sigma : \sigma}{2\eta} + \frac{\sigma : \overset{\triangledown}{\sigma}}{2G}$$

Dissipation? Rate of change of elastic energy?

Oldroyd B model - ICC

Thermodynamic considerations

$$e(\delta,\ \rho,\ \mathbb{B}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}}) = e_0(\delta,\ \rho) + \frac{G}{2\rho}(\mathrm{tr}\mathbb{B}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}} - 3 - \log\det\mathbb{B}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}})$$

$$\longrightarrow \zeta = (\mathbb{T} - G(\mathbb{B}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}} - \mathbb{I}))^{\mathrm{d}} : \mathbb{D}^{\mathrm{d}} + G(\mathbb{C}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}} - \mathbb{I}) : \mathbb{D}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}}$$

Prescribed dissipation

$$\zeta = 2\eta_2|\mathbb{D}|^2 + 2\eta\mathbb{D}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}}\mathbb{C}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}} : \mathbb{D}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}}$$

Resulting model

$$\mathbb{T} = -p\mathbb{I} + 2\eta_2\mathbb{D} + G(\mathbb{B}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}} - \mathbb{I})$$

$$\overset{\triangledown}{\mathbb{B}}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}} = -\frac{G}{\eta}(\mathbb{B}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}} - \mathbb{I})$$

After setting $\eta_2 = 0$, we get Maxwell model

$$\mathbb{T} = -p\mathbb{I} + G(\mathbb{B}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}} - \mathbb{I}) \qquad \mathbb{T} = -p\mathbb{I} + \sigma$$

$$\overset{\triangledown}{\mathbb{B}}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}} = -\frac{G}{\eta}(\mathbb{B}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}} - \mathbb{I}) \qquad \sigma + \tau_{\mathrm{rel}} \overset{\triangledown}{\sigma} = 2\eta\mathbb{D}$$

But now we now the dissipation of our model, we prescribed it

$$\zeta = 2\eta\mathbb{D}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}} \mathbb{C}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}} : \mathbb{D}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}}$$

So the question is

$$2\eta\mathbb{D}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}} \mathbb{C}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}} : \mathbb{D}_{\mathcal{K}_{\mathrm{p}(\mathrm{t})}} \overset{?}{=} \frac{\sigma : \sigma}{2\eta}$$

By using $\sigma = 2\eta\mathbb{D} - \tau_{\mathrm{rel}} \overset{\triangledown}{\sigma}$ and $\sigma = G(\mathbb{B}_{\mathcal{K}_{\mathrm{p}}(\mathrm{t})} - \mathbb{I})$, this question reduces to (kinematic consideration regarding the natural configuration needed):

$$\left(\mathbb{F}_{\mathcal{K}_{\mathrm{p}}(\mathrm{t})}\,\mathbb{D}_{\mathcal{K}_{\mathrm{p}}(\mathrm{t})}\,\mathbb{F}^{\mathrm{T}}_{\mathcal{K}_{\mathrm{p}}(\mathrm{t})}\right) : \left(\mathbb{F}_{\mathcal{K}_{\mathrm{p}}(\mathrm{t})}\,\mathbb{D}_{\mathcal{K}_{\mathrm{p}}(\mathrm{t})}\,\mathbb{F}^{\mathrm{T}}_{\mathcal{K}_{\mathrm{p}}(\mathrm{t})}\right) \overset{?}{=}$$
$$\overset{?}{=} \left(\mathbb{D}_{\mathcal{K}_{\mathrm{p}}(\mathrm{t})}\,\mathbb{F}^{\mathrm{T}}_{\mathcal{K}_{\mathrm{p}}(\mathrm{t})}\,\mathbb{F}_{\mathcal{K}_{\mathrm{p}}(\mathrm{t})}\right) : \mathbb{D}_{\mathcal{K}_{\mathrm{p}}(\mathrm{t})}$$

which is clearly not satisfied

Conclusions

- We used a grid based method to implement viscoelastic rheology into a simple thermal convection model
- Time step decoupling which could be trusted in realistic cases was proposed
- Simulations show that locally high stresses are produced by viscoelasticity, which means that viscoelasticity could trigger plasticity in visco-elasto-plastic code

Thank you