Deriving the equation 00 000000

## Viscoelasticity in mantle convection

## Mgr. et Mgr. Vojtěch Patočka Supervised by: RNDr. Ondřej Čadek, CSc.

Charles University in Prague

[patocka@karel.troja.mff.cuni.cz]

5th June 2015

同 ト イ ヨ ト イ ヨ ト

Testing		Deriving the equation
	000 00000000 00000	00 00000

## Content

### Method of implementation Model Method

#### Testing the method

Thermal convection Mechanical deformation

#### Results

Numerically instaneous behaviour Time step decoupling Elastic episodes

### Construction of the constitutve equation

3D analogs Entropy production maximization



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

글 🖌 🖌 글 🕨

Implementation		
000	000 00000000 00000	00 000000

## Extended Boussinesq - nondimensionalised

### equation of motion + continuity + thermal equation

$$-\nabla \rho + \nabla \cdot \sigma = -\operatorname{Ra} T \vec{e_z}$$
$$\nabla \cdot \vec{v} = 0$$
$$\frac{\partial T}{\partial t} = \nabla^2 T - \vec{v} \cdot \nabla T$$

### rheology

$$\sigma + \mathcal{D} \, \overset{\nabla}{\sigma} = 2\eta \mathbb{D}$$
  
 $\eta(p, T) = \exp(-A(T - T_{ref}) + B(p - p_{ref}))$ 

Implementation		
0 000	000 00000000 00000	00 000000
Method		

### Constitutive equation

$$\sigma + \mathcal{D} \,\overline{\sigma} = 2\eta \mathbb{D} \qquad \mathcal{D}(p, T) := \tau_{\mathrm{rel}} \frac{\kappa}{h^2} = \frac{\eta \kappa}{Gh^2}$$
$$\overline{\sigma} := \frac{\partial \sigma}{\partial t} + (\vec{v} \nabla) \,\sigma + (\sigma \mathbb{W} - \mathbb{W} \sigma) - \mathrm{a}(\mathbb{D}\sigma + \sigma \mathbb{D})$$
advection co-rotation co-deformation

Discretization (mixed euler, 1st order accurate)

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

Implementation		
0 0●0	000 00000000 00000	00 000000
Method		

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

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

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

Viscoelasticity parameter  ${\rm Z}$ 

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

<ロト <問 > < 注 > < 注 >

Implementation
000

Testing 0000 Results 000 000000000 00000 Deriving the equation 00 000000

## $dt^{n-1,n} = \text{stability}(\vec{v}^{n-1}, \mathcal{D}, d); \quad dt^{a}; \quad dt^{el}$ $T^{n} =$ advection-diffusion ( $T^{n-1}, \vec{v}^{n-1}, dt^{a}$ ) no decoupling: $\tilde{\sigma}^{n-1} = \sigma^{n-1} + \text{deadvection} (\sigma^{n-1}, \vec{v}^{n-1}, dt^a)$ $dt^{a} = dt^{n-1, n}$ $\eta^{n} = \eta(T^{n});$ $\eta^{n}_{num} = \eta^{n}_{num}(\eta^{n}, dt^{el}, \mathcal{D}^{n})$ $dt^{el} = dt^{n-1, n}$ $\mathsf{rhs}^{\mathrm{n}} = \nabla \cdot \left( \frac{\mathcal{D}^{n}}{\mathrm{d}t^{\mathrm{el}} + \mathcal{D}^{n}} \, \tilde{\sigma}^{n-1} \right) - \operatorname{Ra} \mathcal{T}^{\mathrm{n}} \, \vec{e_{z}}$ $Stokes(\eta_{num}^n, \vec{v}^n, p^n) = rhs^n$ $\sigma^n = \sigma^n (\tilde{\sigma}^{n-1}, \eta_{\text{num}}^n, \vec{v}^n)$

#### Viscoelasticity in mantle convection

#### Charles University in Prague

同 ト イヨ ト イヨ ト ヨ うくで



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:  $\mu(75, 275, ..., 1075)$ .

Viscoelasticity in mantle convection

Charles University in Prague

79

Testing 0●00 Results 000 000000000 00000 Deriving the equation 00 000000

Thermal convection

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





▲圖 ▶ ▲ 臣 ▶ ▲ 臣 ▶

э

Testing 00●0 Results 000 000000000 00000 Deriving the equation 00 000000

Thermal convection

## Upper convected derivative (a = 1)





<ロ> <同> <同> < 同> < 同>

#### Viscoelasticity in mantle convection

#### Charles University in Prague

э

	Testing 000● 0	<b>Results</b> 000 000000000 00000	Deriving the equation 00 000000
Thermal convection			

### Viscous case





<ロ> <同> <同> < 同> < 同>

æ

Testing		Deriving the equation
0000 <sup>°</sup>	000 00000000 00000	00 000000

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

$$\rho_1 = 4000; \quad \eta_1 = 1 \text{ e27}; \quad G_1 = 1 \text{ e10};$$
  
 $\rho_2 = 1; \quad \eta_2 = 1 \text{ e21}; \quad G_2 = 1 \text{ e20};$ 



Charles University in Prague

・ 同 ト ・ ヨ ト ・ ヨ ト



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



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

-

Image: A image: A

		Results	Deriving the e
		<b>000</b> 00000000 00000	00
Numerically instaneous behave	viour		

### Example of velocity singularity



Viscoelasticity in mantle convection

э

<ロ> <同> <同> < 同> < 同>

Testing 0000 Results 00● 000000000 00000 Deriving the equation 00 000000

Numerically instaneous behaviour

## Jaumann - parametric study, failed runs



#### Charles University in Prague

э

Implementation 0 000 Testing 0000 Results

Deriving the equation 00 000000

Time step decoupling

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

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

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

$$\eta^{n} = \eta(T^{n}); \quad \eta^{n}_{num} = \eta^{n}_{num}(\eta^{n}, dt^{el}, \mathcal{D}^{n})$$

$$\downarrow$$

$$rhs^{n} = \nabla \cdot \left(\frac{\mathcal{D}^{n}}{dt^{el} + \mathcal{D}^{n}} \tilde{\sigma}^{n-1}\right) - \text{Ra} T^{n} \vec{e_{z}}$$

$$\downarrow$$

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

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

#### Viscoelasticity in mantle convection

э.

・ロン ・部 と ・ ヨ と ・ ヨ と …

Implementation 0 000 Testing 0000 Results 000 000000000 000000000 Deriving the equation 00 000000

 $dt^{n-1,n} = \text{stability}(\vec{v}^{n-1}, \mathcal{D}, d); \quad dt^{a}; \quad dt^{el}$  $T^{n} =$ advection-diffusion ( $T^{n-1}, \vec{v}^{n-1}, dt^{a}$ ) convection  $\tilde{\sigma}^{n-1} = \sigma^{n-1} + \text{deadvection} (\sigma^{n-1}, \vec{v}^{n-1}, dt^a)$ decoupling:  $\eta^{n} = \eta(T^{n});$   $\eta^{n}_{num} = \eta^{n}_{num}(\eta^{n}, dt^{el}, \mathcal{D}^{n})$  $\mathsf{rhs}^{\mathrm{n}} = \nabla \cdot \left( \frac{\mathcal{D}^{n}}{\mathrm{d}t^{\mathrm{el}} + \mathcal{D}^{n}} \, \tilde{\sigma}^{n-1} \right) - \operatorname{Ra} \mathcal{T}^{\mathrm{n}} \, \vec{e_{z}}$ interpolation needed  $Stokes(\eta_{num}^{n}, \vec{v}^{n}, p^{n}) = rhs^{n}$  $\sigma^n = \sigma^n (\tilde{\sigma}^{n-1}, \eta_{\text{num}}^n, \vec{v}^n)$ 

Charles University in Prague

同 ト イヨ ト イヨ ト ヨ うくで



Realistic case: separate viscous and viscoelastic parts of the domain

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

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

伺 ト く ヨ ト く ヨ ト

Testin 0000 Results

Deriving the equation 00 000000

Time step decoupling

## Jaumann - failed runs, decoupled



Viscoelasticity in mantle convection

Charles University in Prague

Testing

Results

Deriving the equation 00 000000

Time step decoupling

## Upper convected - failed runs, decoupled



Charles University in Prague

э

Testing

Results

Deriving the equation 00 000000

## Jaumann - not "trusted" runs, decoupled



Charles University in Prague

3

	Results ○○○ ○○○○○○○○○○○○○○○○○○○○○○○○○○○○○○○○	Deriving the equation 00 000000
Time step decoupling		

### Critical Deborah, time step decoupled





#### Critical Deborah, time step decoupled: elastic strain rate



э

イロン イロン イヨン イヨン



### Critical Deborah, time step decoupled: upper convected



э

イロン イロン イヨン イヨン

	Results 000 00000000 ●0000	Deriving the equation 00 000000



æ

	Testing	Results	Deriving the equation
		000 00000000 0●000	00 000000
Elastic episodes			

### Undercritical Deborah number - time step/scheme convergence



#### Viscoelasticity in mantle convection

Charles University in Prague

э

Testing	Results	Deriving the equation
	000 00000000 00000	00 000000

### Overcritical Deborah number - time step convergence



#### Viscoelasticity in mantle convection

#### Charles University in Prague

э

3

	Results 000 00000000 000●0	Deriving the equation 00 000000
Elastic episodes		

### Overcritical Deborah number - time scheme convergence



Viscoelasticity in mantle convection

#### Charles University in Prague

э

⊸ ≣ ⊁

<⊡> <≣

	Testing	Results	Deriving the equation
		000 00000000 <b>0000</b>	00 000000
Elactic opicodos			

Time step analysis - overcritical Deborah number



э

▲□ ▶ ▲ □ ▶ ▲ □ ▶

Testing 0000 0 Results 000 000000000 00000 Deriving the equation

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 ...

A 3 b

	Testing		Deriving the equation
		000 00000000 00000	<b>0</b> 00000
3D analogs			

## 3D analogs

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

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

$$egin{aligned} &arepsilon^{\mathrm{lin}} :=& rac{1}{2} \left( 
abla u + (
abla u)^{\mathrm{T}} 
ight); & \xi^{\mathrm{lin}} :=& rac{1}{2} \left( \mathrm{Grad} U + (\mathrm{Grad} U)^{\mathrm{T}} 
ight) \ &arepsilon :=& rac{1}{2} (\mathbb{I} - \mathbb{F}^{-\mathrm{T}} \mathbb{F}^{-1}); & \xi :=& rac{1}{2} \left( \mathbb{F}^{\mathrm{T}} \mathbb{F} - \mathbb{I} 
ight) \end{aligned}$$

which have following material time derivatives

$$egin{aligned} \dot{arepsilon}^{\mathrm{lin}} &= \mathbb{D} - rac{1}{2} ((
abla u) \mathbb{L} + \mathbb{L}^{\mathrm{T}} (
abla u)^{\mathrm{T}}) & \dot{arepsilon} &= \mathbb{D} - (arepsilon \mathbb{L} + \mathbb{L}^{\mathrm{T}} arepsilon) \ \dot{arepsilon}^{\mathrm{lin}} &= \mathbb{D} - rac{1}{2} ((
abla u)^{\mathrm{T}} \mathbb{L}^{\mathrm{T}} + \mathbb{L} (
abla u)) & \dot{arepsilon} &= \mathbb{F}^{\mathrm{T}} \, \mathbb{D} \, \mathbb{F} \end{aligned}$$



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

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

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

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

・ 同 ト ・ ヨ ト ・ ヨ ト …

Results 000 000000000 00000 Deriving the equation  $\circ\circ$  $\circ\circ\circ\circ\circ\circ\circ\circ$ 

#### Rajagopal

## Entropy production maximization

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

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

Dissipation? Rate of change of elastic energy?

∃ ▶ ∢

		Deriving the equation
	000 00000000 00000	00000
Rajagonal		

## Oldroyd B model - ICC

Thermodynamic considerations

٣

$$\begin{split} e(\delta, \, \rho, \, \mathbb{B}_{\mathcal{K}_{\mathrm{p}}(\mathrm{t})}) &= e_{0}(\delta, \, \rho) + \frac{G}{2\rho}(\mathrm{tr}\mathbb{B}_{\mathcal{K}_{\mathrm{p}}(\mathrm{t})} - 3 - \log \det \mathbb{B}_{\mathcal{K}_{\mathrm{p}}(\mathrm{t})}) \\ &\longrightarrow \zeta = (\mathbb{T} - G(\mathbb{B}_{\mathcal{K}_{\mathrm{p}}(\mathrm{t})} - \mathbb{I}))^{\mathrm{d}} : \mathbb{D}^{\mathrm{d}} + G(\mathbb{C}_{\mathcal{K}_{\mathrm{p}}(\mathrm{t})} - \mathbb{I}) : \mathbb{D}_{\mathcal{K}_{\mathrm{p}}(\mathrm{t})}) \end{split}$$

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

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

$$\stackrel{\scriptscriptstyle 
olymbol {
extstyle}}{\mathbb{B}}_{\mathcal{K}_{\mathrm{p}}(\mathrm{t})} = -rac{\mathsf{G}}{\eta}(\mathbb{B}_{\mathcal{K}_{\mathrm{p}}(\mathrm{t})} - \mathbb{I})$$

Testing		Deriving the equation
	000 00000000 00000	000000

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

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

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



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

$$(\mathbb{F}_{\mathcal{K}_{p}(t)} \mathbb{D}_{\mathcal{K}_{p}(t)} \mathbb{F}_{\mathcal{K}_{p}(t)}^{T}) : (\mathbb{F}_{\mathcal{K}_{p}(t)} \mathbb{D}_{\mathcal{K}_{p}(t)} \mathbb{F}_{\mathcal{K}_{p}(t)}^{T}) \stackrel{?}{=} \\ \stackrel{?}{=} (\mathbb{D}_{\mathcal{K}_{p}(t)} \mathbb{F}_{\mathcal{K}_{p}(t)}^{T} \mathbb{F}_{\mathcal{K}_{p}(t)}) : \mathbb{D}_{\mathcal{K}_{p}(t)}$$

which is clearly not satisfied

伺 ト く ヨ ト く ヨ ト

		Deriving the equation
	000 00000000 00000	0000000
Rajagonal		

## 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

		Deriving the equation
	000 00000000 00000	00 00000
Raiagonal		

# Thank you