A Multigrid LCR-FEM solver for viscoelastic fluids with application to problems with free surface

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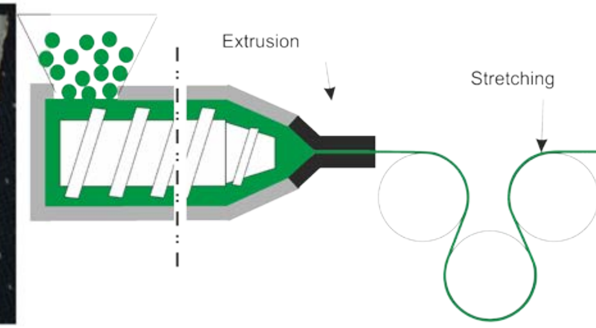
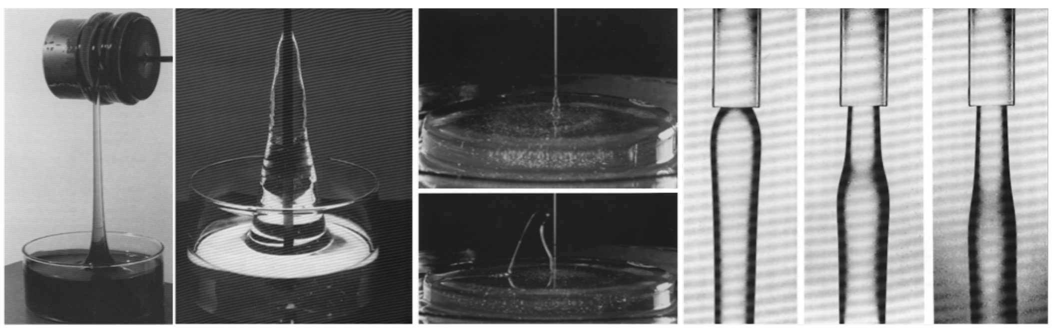
(Lausanne, August 2013)

Polymer melts:

- One of industrial interests +
- Physically fascinating +
- Rheologically difficult -
- Numerically challenging -





Highly accurate, robust numerical solver which represents the rheological nature is still challenging

Viscoelastic fluid models **(D. D. Joseph)**:

- Integral form

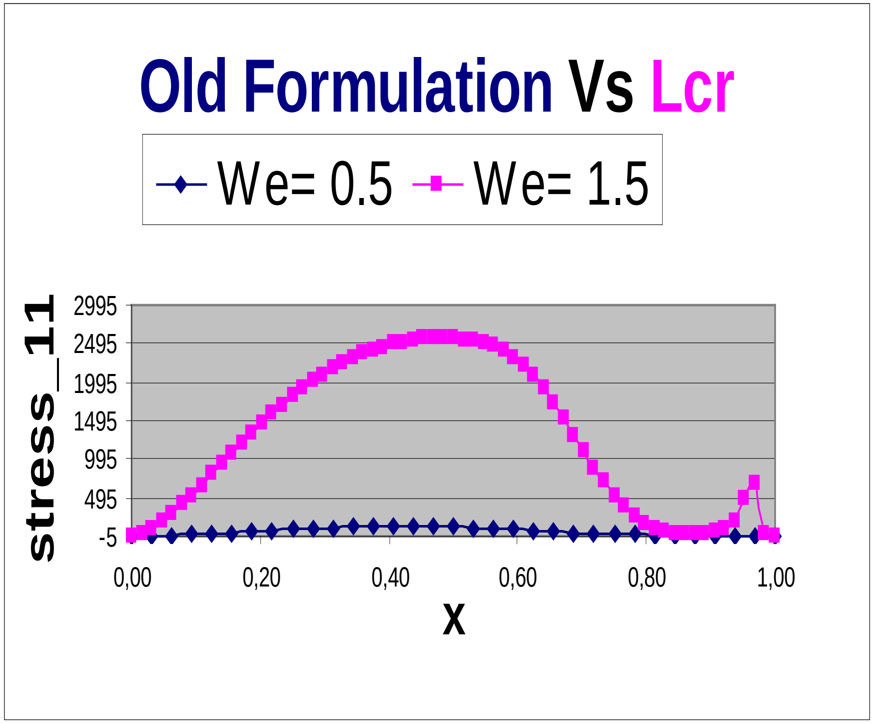
$$\tau(t) = \int_{-\sim}^{t} \frac{1}{We^2} e^{\frac{-(t-s)}{We}} F(s,t)F(s,t)^T \, ds$$

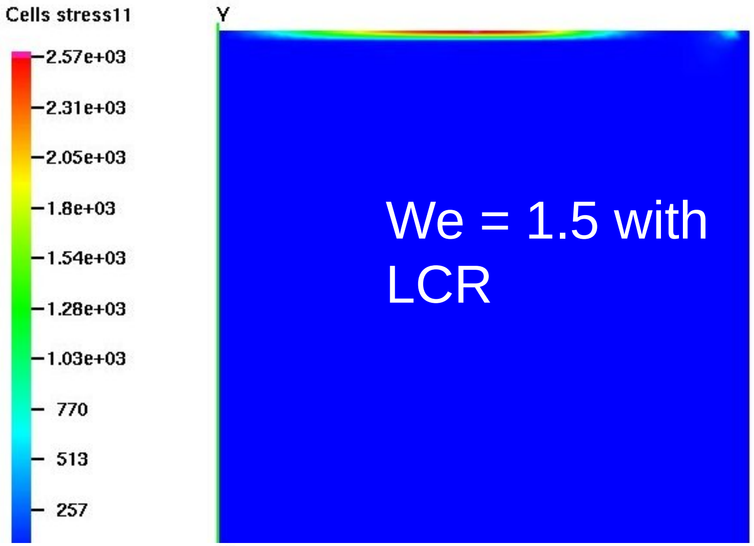
- Differential form: Upper-convected derivative
- More practical to implement than integral form
- Represent many viscoelastic models

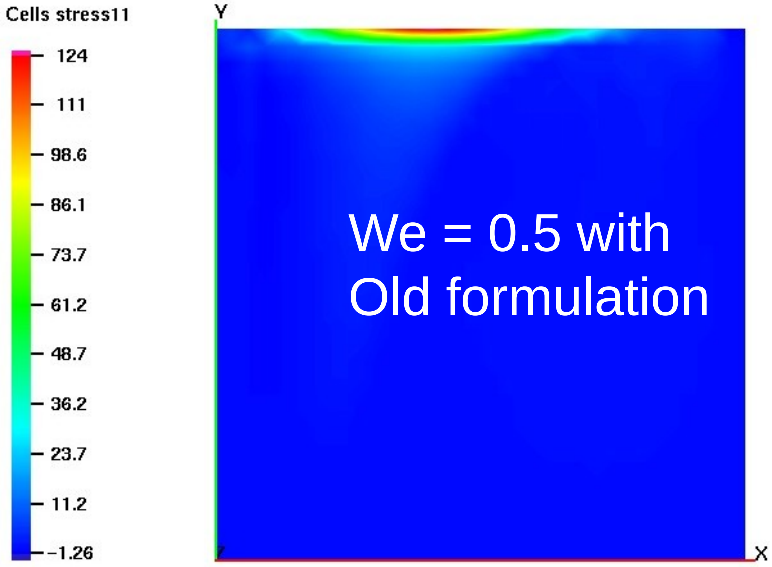
$$\frac{\partial \tau}{\partial t} + (u \cdot \nabla)\tau - \nabla u \cdot \tau - \tau \cdot \nabla u^T = f(\tau)$$

- Conformation tensor (τ), velocity (u), source ($f(\tau)$)
- Not able to capture high stress gradient at higher We number
- $f(\tau)$ can be Oldroyd-B, Giesekus, FENE, PTT, WM, Pom-Pom

Cutline of Stress_11
component at y = 1.0







Experience **(Kupferman et. al)**:

- Stresses grow exponentially
- Conformation tensor looses positive properties during numerics

$$\frac{\partial \tau}{\partial t} + (u \cdot \nabla)\tau - \nabla u \cdot \tau - \tau \cdot \nabla u^T = f(\tau)$$

$$\nabla u = \Omega + B + N\tau^{-1}$$

$$\frac{\partial \tau}{\partial t} + (u \cdot \nabla)\tau - (\Omega\tau - \tau\Omega) - 2B\tau = f(\tau)$$

$$\tau = e^{\psi}$$

$$\frac{\partial \psi}{\partial t} + (u \cdot \nabla)\psi - (\Omega\psi - \psi\Omega) - 2B = g(\psi)$$

LCR based models

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LCR based viscoelastic fluid:

- Ability to capture high stress gradients at higher We number
- Positivity preserving by design $\tau = e^{\psi}$
- Numerically more stable with appropriate FEM

$$\frac{\partial \psi}{\partial t} + (u \cdot \nabla)\psi - (\Omega\psi - \psi\Omega) - 2B = g(\psi)$$

- LCR tensor (ψ), velocity (u), source ($g(\psi)$)
- $\nabla u = \Omega + B + N\tau^{-1}$
- $g(\psi)$can be Oldroyd-B, Giesekus, FENE, PTT, WM, Pom-Pom

LCR based viscoelastic fluid:

Model	$f(\boldsymbol{\tau})$	$g(\boldsymbol{\psi})$
OdB	$1/\lambda(\mathbf{I}-\boldsymbol{\tau})$	$1/\lambda\,(\exp(-\boldsymbol{\psi})-\mathbf{I})$
Gie	$1/\lambda\,(\mathbf{I}-\boldsymbol{\tau}-\alpha(\boldsymbol{\tau}-\mathbf{I})^2)$	$1/\lambda\,(\exp(-\boldsymbol{\psi})-\mathbf{I})-\alpha\exp(\boldsymbol{\psi})(\exp(-\boldsymbol{\psi})-\mathbf{I})^2)$
FENE	$-1/\lambda\,(f(R)\boldsymbol{\tau}-\alpha f(R)\mathbf{I})$	$-1/\lambda\,(f(R)-\alpha f(R)\exp(-\boldsymbol{\psi}))$
LPTT	$-1/\lambda\,(1+\varepsilon(\mathrm{tr}(\boldsymbol{\tau})-3))(\mathbf{I}-\boldsymbol{\tau})$	$-1/\lambda\,(1+\varepsilon(\mathrm{tr}(\exp(\boldsymbol{\psi}))-3))(\exp(-\boldsymbol{\psi})-\mathbf{I})$
XPTT	$-1/\lambda\,(\exp(\varepsilon(\mathrm{tr}(\boldsymbol{\tau})-3)))(\mathbf{I}-\boldsymbol{\tau})$	$-1/\lambda\,(\exp(\varepsilon(\mathrm{tr}(\exp(\boldsymbol{\psi}))-3)))(\exp(-\psi)-\mathbf{I})$
WM	$-1/\lambda(\dot{\gamma})\,(\boldsymbol{\tau}-\mathbf{I})$	$-1/\lambda(\dot{\gamma})\,(\mathbf{I}-\exp(-\boldsymbol{\psi}))$
Pom	$-1/\lambda_{\mathbf{b}}(f(\boldsymbol{\tau})-2\alpha+\alpha\boldsymbol{\tau}+(\alpha-1)\mathbf{I})$	$-1/\lambda_{\mathbf{b}}(f(\boldsymbol{\psi})-2\alpha+\alpha\exp(\boldsymbol{\psi})+(\alpha-1)\exp(-\boldsymbol{\psi}))$

- Relaxation time (λ)

Multiphysics flow model

- Navier-Stokes equation (u, p)

$$\rho\left(\frac{\partial}{\partial t} + u \cdot \nabla\right) u = -\nabla p + \nabla \cdot \sigma_s + \frac{1}{\lambda} \nabla \cdot \eta_p e^{\psi}, \qquad \nabla \cdot u = 0$$

- \+ Nonlinear viscosities

$$\sigma_s = 2\eta_s(\dot{\gamma}, \Theta, p) D, \ \dot{\gamma} = \sqrt{tr(D^2)}$$

- \+ Temperature effects with Boussinesq and viscous dissipation (Θ)

$$\rho c_p\left(\frac{\partial}{\partial t} + u \cdot \nabla\right)\Theta = k_1 \nabla^2 \Theta + k_2 D : D$$

- \+ Viscoelastic fluid models (ψ)

$$\frac{\partial \psi}{\partial t} + (u \cdot \nabla)\psi - (\Omega\psi - \psi\Omega) - 2B = g(\psi)$$

- \+ Multiphase flow with Level-Set equation

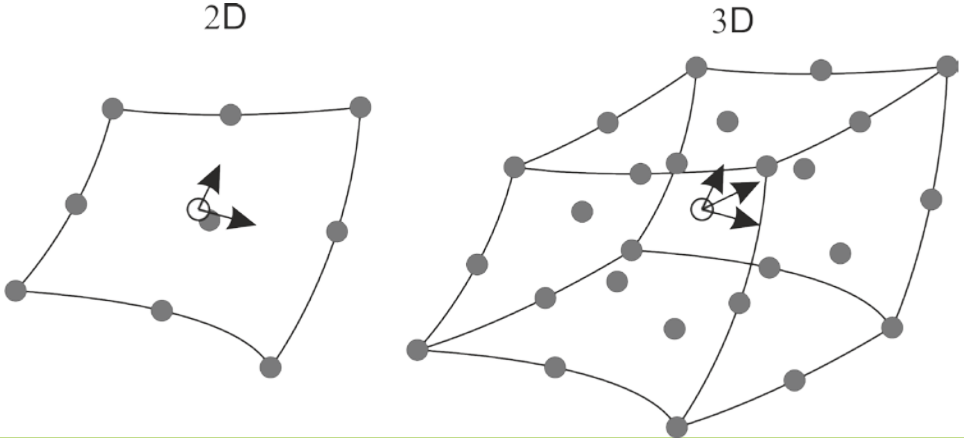
$$\frac{\partial \varphi}{\partial t} + (u \cdot \nabla)\varphi = 0$$

In Time:

- Second order Crank-Nicolson
- Can be adaptively applied

In Space: Higher order finite element **(Arnoldi)**

- Inf-sup stable for velocity and pressure
- High order: good for accuracy
- Discontinuous pressure: good for solver & physics
- Edge oriented FEM for numerical stabilitation **(Burman)**



Discrete system

Saddle point problem:

- $\tilde{u}$ consists of all numerical variables except pressure
- Newton with multigrid as well-known solver
- Monolithic way of solving

$$\begin{pmatrix} A & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} \tilde{u} \\ p \end{pmatrix} = \begin{pmatrix} \mathrm{rhs}_{\tilde{u}} \\ \mathrm{rhs}_p \end{pmatrix}$$

- A consists of differential operators
- B is gradient operator

Newton iteration

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Newton for nonlinear system:

- Strongly coupled problem
- Automatic damping control ω^n for each nonlinear step
- Black-box for many given viscoelastic models

$$x^{n+1} = x^n + \omega^n \left[\frac{\partial \mathcal{R}(x^n)}{\partial x} \right]^{-1} \mathcal{R}(x^n)$$

- Quadratic convergence when iterative solutions are close
- Solution $x^{n+1} = (\tilde{u}, p)$, Residual equation $\mathcal{R}(x^n)$
- Black-box is made possible by divided difference technique

$$\left[\frac{\partial \mathcal{R}(x^n)}{\partial x} \right]_{ij} = \frac{\mathcal{R}_i\left(x^n + \varepsilon e_j\right) - \mathcal{R}_i\left(x^n + \varepsilon e_j\right)}{2\varepsilon}$$

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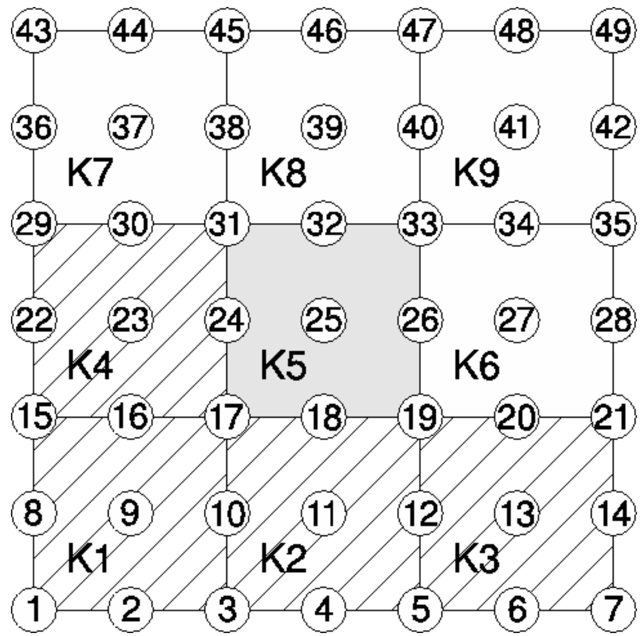
Multigrid for linearized system:

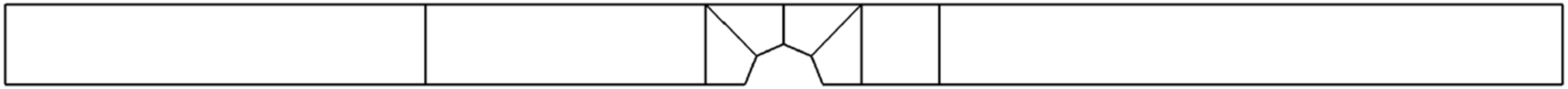
- Full-Vanka for strongly coupled Jacobian in local system
- Full prolongation
- Black-box for many given viscoelastic models

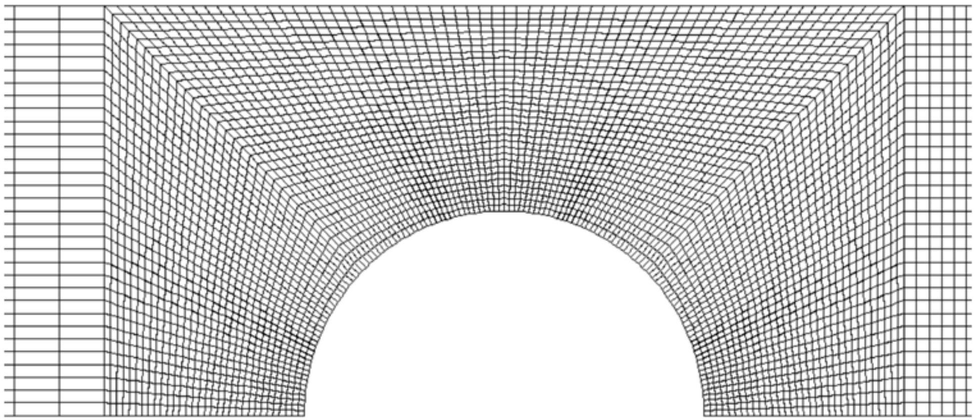


$$\begin{bmatrix}\tilde{u}^{l+1}\\ p^{l+1}\end{bmatrix} = \begin{bmatrix}\tilde{u}^{l}\\ p^{l}\end{bmatrix} \text{"} + \text{"} \omega \sum_{\text{patch } \Omega_i} \begin{bmatrix} A_{\tilde{u}|\Omega_i} & kB_{|\Omega_i}\\ {B^T}_{|\Omega_i} & 0\end{bmatrix}^{-1} \begin{bmatrix}\text{def}_{\tilde{u}|\Omega_i}\\ \text{def}_{p|\Omega_i}\end{bmatrix}$$

Numerical examples 1

Flow around cylinder:





Level	NEL	DOF
R1	32	921
R2	128	3309
R3	512	12501
R4	2048	48549
R5	8192	191301
R6	32768	759429

Mod.	**Gie**	**FENE-P**	**FENE-C**	**WM-Lr**	**WM-Cr**	**WM-Ca**	**LPPT/ XPPT**	**Pom**
Par	α=0.01	α = 0, L2=100	α = 1, L2=100	l=0.01	k=0.01, l=0.01, m=0.01, n=0.01	a = 0.95, b = 0.95, k= 0.01, l = 0.01, m = 0.01, n = 0.01	ε=0.01	α=0.01, v = 0.2, r = 1

Numerical examples 1

Flow around cylinder:

Lev.	Oldroyd-B	Giesekus	FENE-P	FENE-CR	LPTT
R1	126.5259[5/1]	126.0070[5/1]	125.3255[5/1]	126.6369[5/1]	126.5436[5/1]
R2	128.9641[5/1]	128.3420[4/1]	127.6645[5/1]	129.0771[5/1]	128.9727[5/1]
R3	129.9711[3/1]	129.2975[3/1]	128.6161[3/1]	130.0719[3/1]	129.9712[3/1]
R4	130.2648[2/2]	129.5757[2/2]	128.8925[2/2]	130.3606[2/2]	130.2608[2/2]
R5	130.3388[2/2]	129.6466[2/2]	128.9632[2/2]	130.4338[2/2]	130.3341[2/2]
	XPTT	**WM-Larson**	**WM-Cross**	**WM-Carreau**	**Pom-Pom**
R1	126.5437[5/1]	126.3346[5/1]	124.6317[5/1]	124.3082[5/1]	126.0887[4/1]
R2	128.9728[5/1]	128.7564[4/1]	126.9133[5/1]	126.5703[5/1]	128.3629[5/1]
R3	129.9713[3/1]	129.7564[3/1]	127.8540[3/1]	127.5025[3/1]	129.1754[3/1]
R4	130.2608[2/2]	130.0482[2/2]	128.1303[2/2]	127.7764[2/2]	129.4095[2/2]
R5	130.3342[2/2]	130.1219[2/2]	128.2007[2/2]	127.8463[2/2]	129.4728[2/2]

Newton-multigrid behaviour for We=0.1

Numerical examples 1

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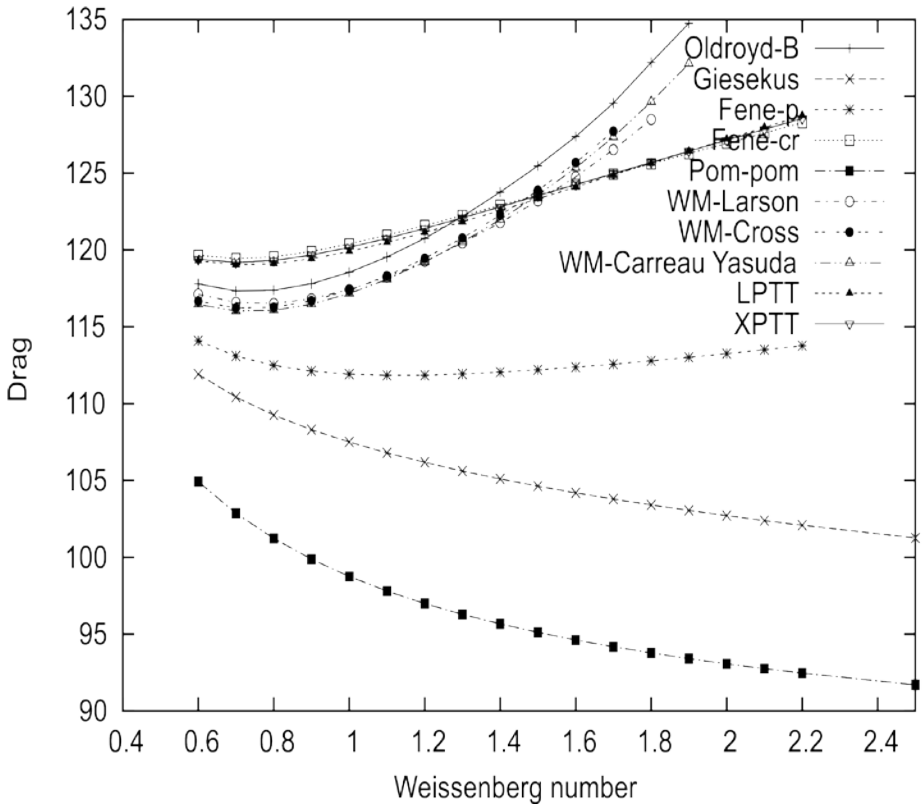
Flow around cylinder:

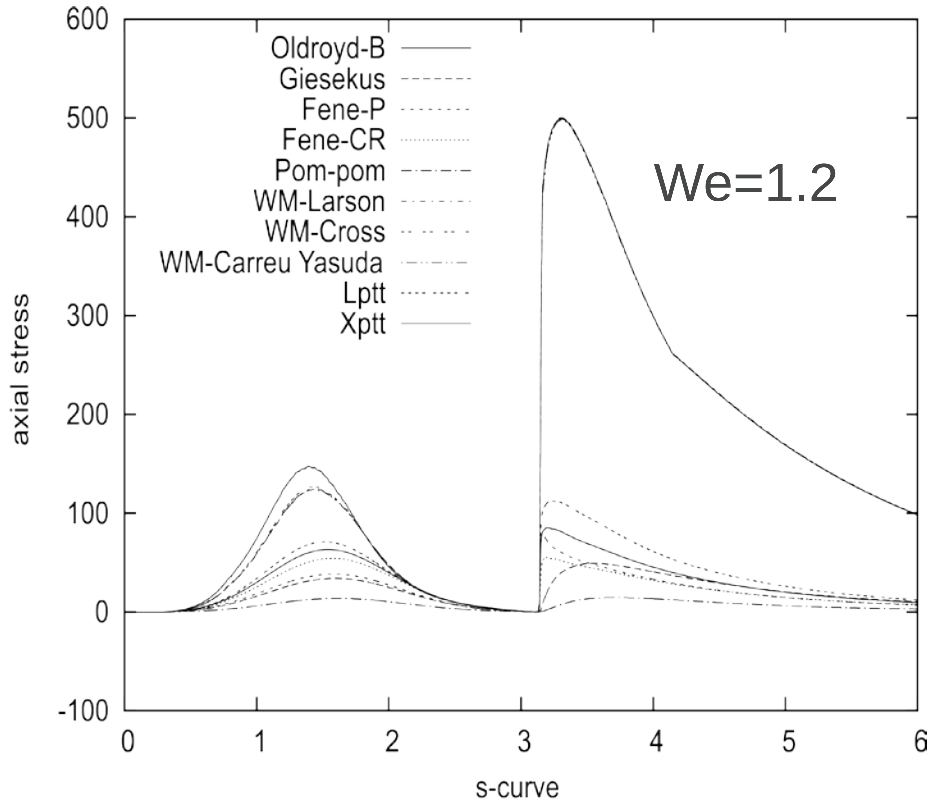
We	Oldroyd-B	Giesekus	FENE-P	FENE-CR	LPTT
0.6	117.7887[2]	111.9109[2]	114.0870[2]	119.6564[2]	119.2840[2]
0.7	117.3345[3]	110.4256[3]	113.1044[3]	119.4340[3]	119.0223[3]
0.8	117.3718[3]	109.2601[3]	112.4831[3]	119.5552[3]	119.1038[3]
0.9	117.8039[4]	108.3084[3]	112.1125[4]	119.9018[4]	119.4197[3]
1.0	118.5410[3]	107.5035[3]	111.9158[4]	120.3899[4]	119.8937[3]
1.1	119.5344[3]	106.8035[3]	111.8408[4]	120.9640[4]	120.4741[3]
1.2	120.7520[5]	106.1817[5]	111.8526[3]	121.5885[3]	121.1270[3]
	XPTT	**WM-Larson**	**WM-Cross**	**WM-Carreau**	**Pom-Pom**
0.6	119.4010[2]	117.1221[2]	116.6605[2]	116.4609[2]	104.9392[4]
0.7	119.1871[3]	116.5785[3]	116.2328[3]	116.0340[3]	102.8783[3]
0.8	119.3129[3]	116.5114[3]	116.2700[3]	116.0675[3]	101.2295[3]
0.9	119.6645[3]	116.8218[4]	116.6810[4]	116.4717[4]	99.8823[3]
1.0	120.1624[3]	117.4164[3]	117.3786[3]	117.1597[3]	98.7611[3]
1.1	120.7540[3]	118.2415[3]	118.3140[3]	118.0826[3]	97.8127[3]
1.2	121.4052[3]	119.2616[3]	119.4559[3]	119.2094[3]	96.9987[4]

Moderate number of nonlinear steps for all models

Numerical examples 1

Flow around cylinder:

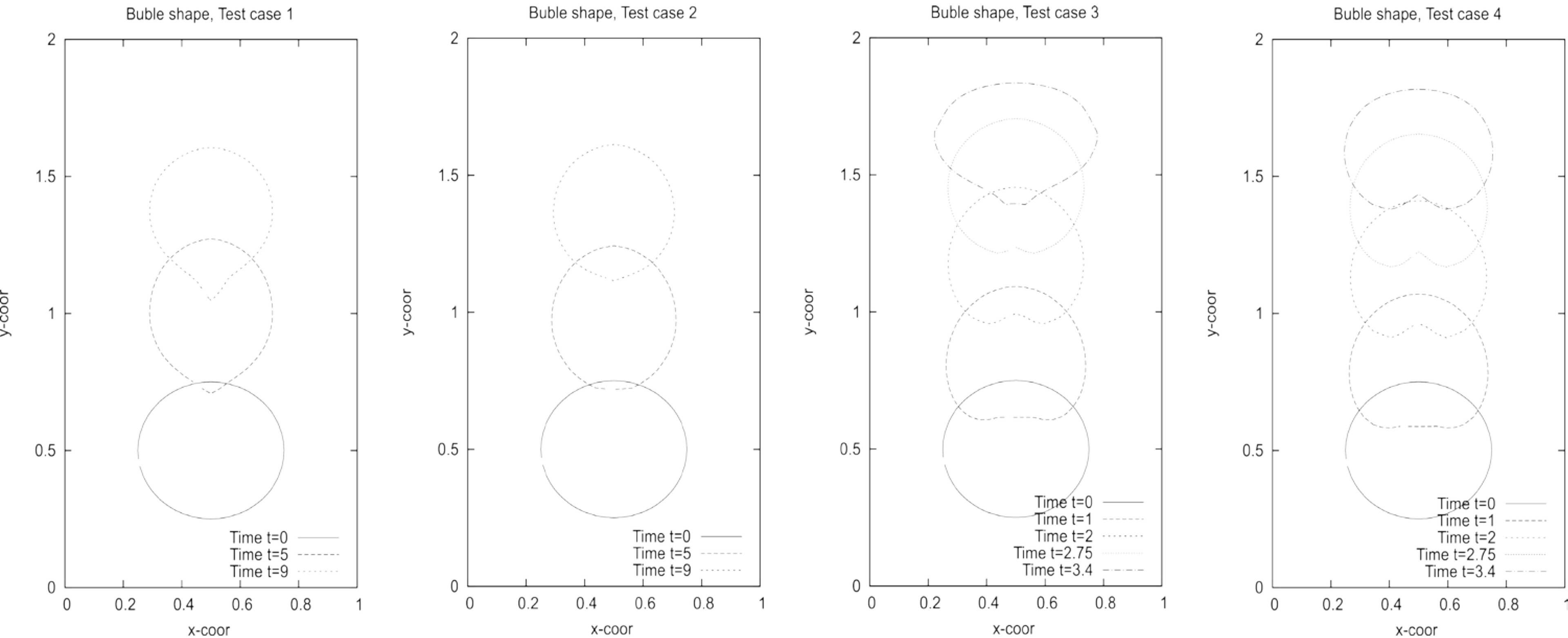




Different drag behaviour of different models at increasing We number

Numerical examples 2

Rising bubble in viscoelastic fluid:

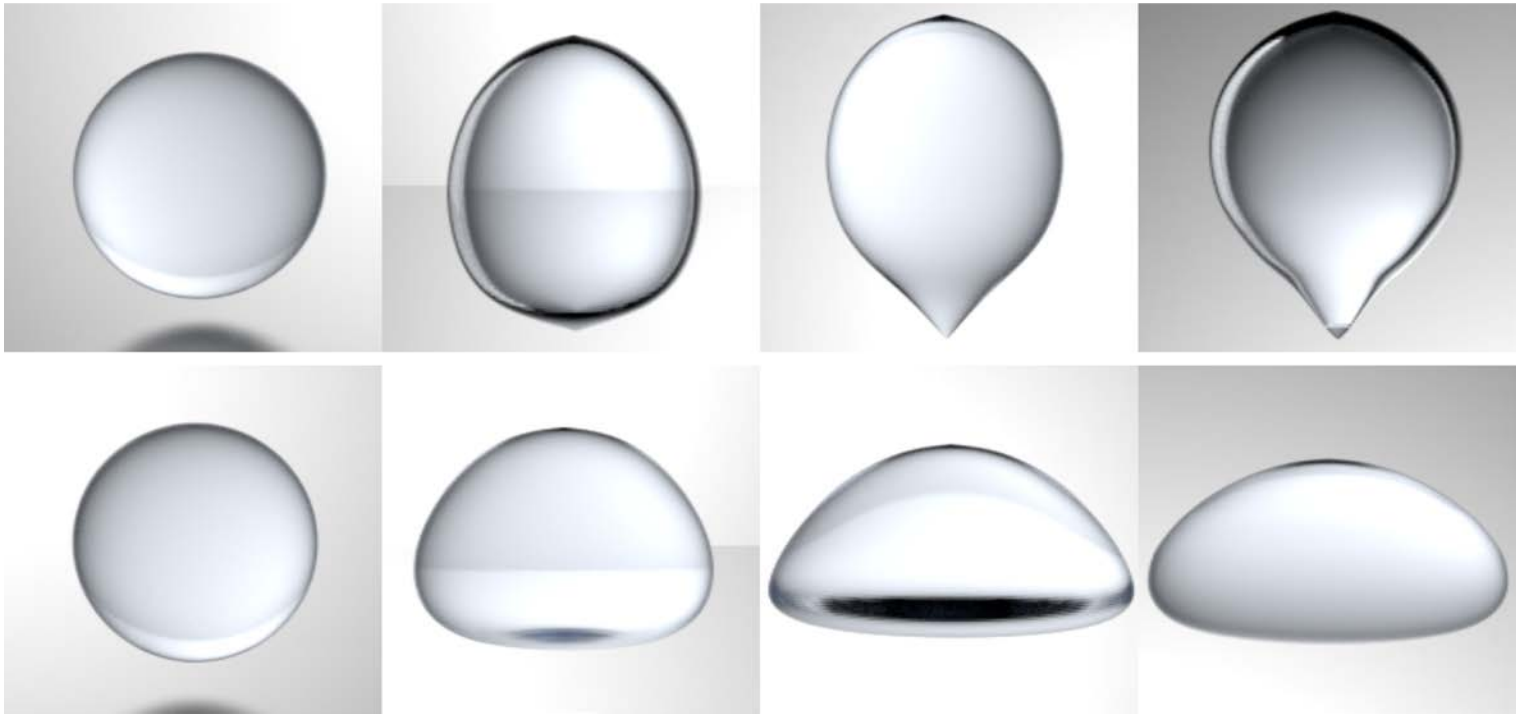


Material 1: Viscoelastic fluid described by the Oldroyd-B model

Material 2: Newtonian fluid

Test case	ρ_1	ρ_2	μ_1	μ_2	$\mathbf{g}$	σ
1. Viscoelastic ($\Lambda = 10$)	10	0.1	10	1	9.8	0.245
2. Newtonian ($\Lambda = 0$)	10	0.1	10	1	9.8	0.245
3. Viscoelastic ($\Lambda = 10$)	10	0.1	2	1	9.8	0.245
4. Newtonian ($\Lambda = 0$)	10	0.1	2	1	9.8	0.245

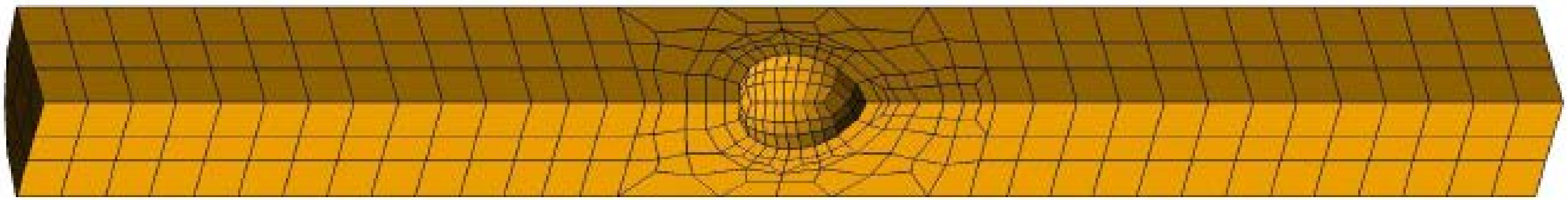
Rising bubble in viscoelastic fluid:



- A better visualisation from the data before. „cheating bubbles“
- Multiphase flow in a cylindrical coordinate system is ongoing

3D flow around a sphere:

- An LCR based FEM solver for 3D viscoelastic flow
- Tests with Oldroyd-B for We=0.3 and 0.6



We=0.3

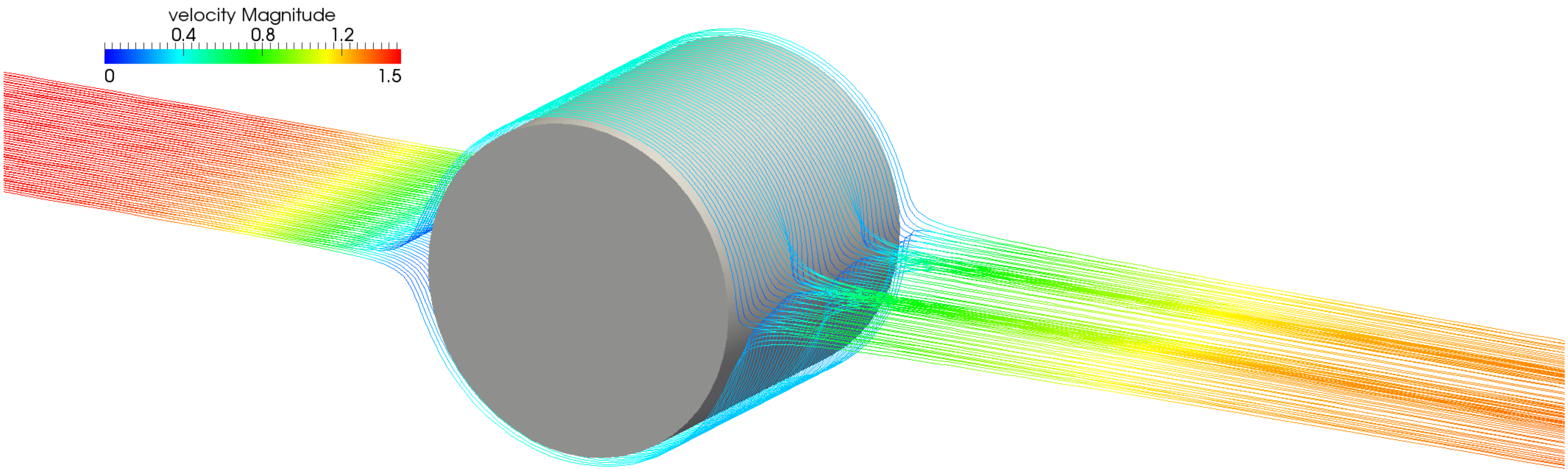
Resolution	$\max_1(\tau_{xx})$	$\max_2(\tau_{xx})$	F^*
L2	20.80	2.082	5.6976
L3	19.29	2.081	5.6946
L4	18.72	2.086	5.6941
L5	18.52	2.087	5.6940
Authors		Reference values	
Lunsmann [4]	-	-	5.6937
Owens [5]	18.27	-	5.6963

We=0.6

Resolution	$\max_1(\tau_{xx})$	$\max_2(\tau_{xx})$	F^*
L2	50.31	5.041	5.4170
L3	39.01	5.061	5.4133
L4	36.43	5.104	5.4128
L5	35.65	5.118	5.4128
Authors		Reference values	
Lunsmann [4]	35.17	-	5.4123
Owens [5]	35.67	-	5.4117
Sahin [6]	34.73	5.12	-

3D flow around cylinder:

- An LCR based FEM solver for 3D viscoelastic flow
- Tests with Oldroyd-B
- Invariance in z-direction for We=1.6, agreement with Sahin et. al



Numerical examples 5

Polymer stretching:

- A 2D+1 membrane model **(Sollogoub et. Al)**

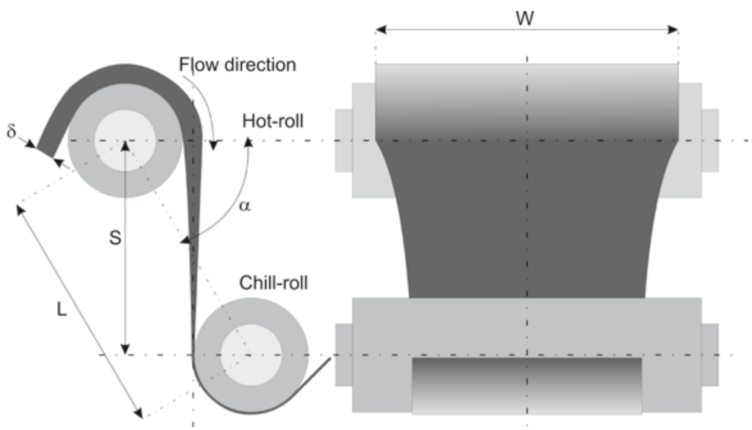
$$\nabla \cdot eU = 0$$

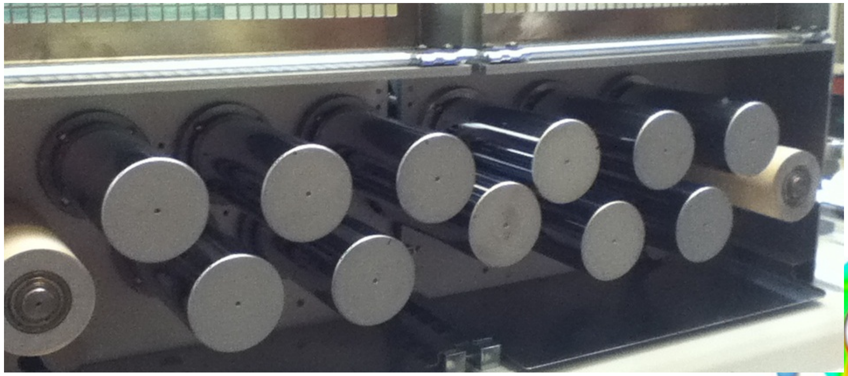
$$\nabla \cdot e(2\mu D + 2\mu\, tr(D)I) = \nabla \cdot e\tau$$

$$\frac{\partial \tau}{\partial t} + (U \cdot \nabla)\tau - \nabla U \cdot \tau - \tau \cdot \nabla U^T = \frac{1}{\lambda} f$$

- Level set-FEM

$$\frac{\partial \varphi}{\partial t} + (U \cdot \nabla)\varphi = 0$$

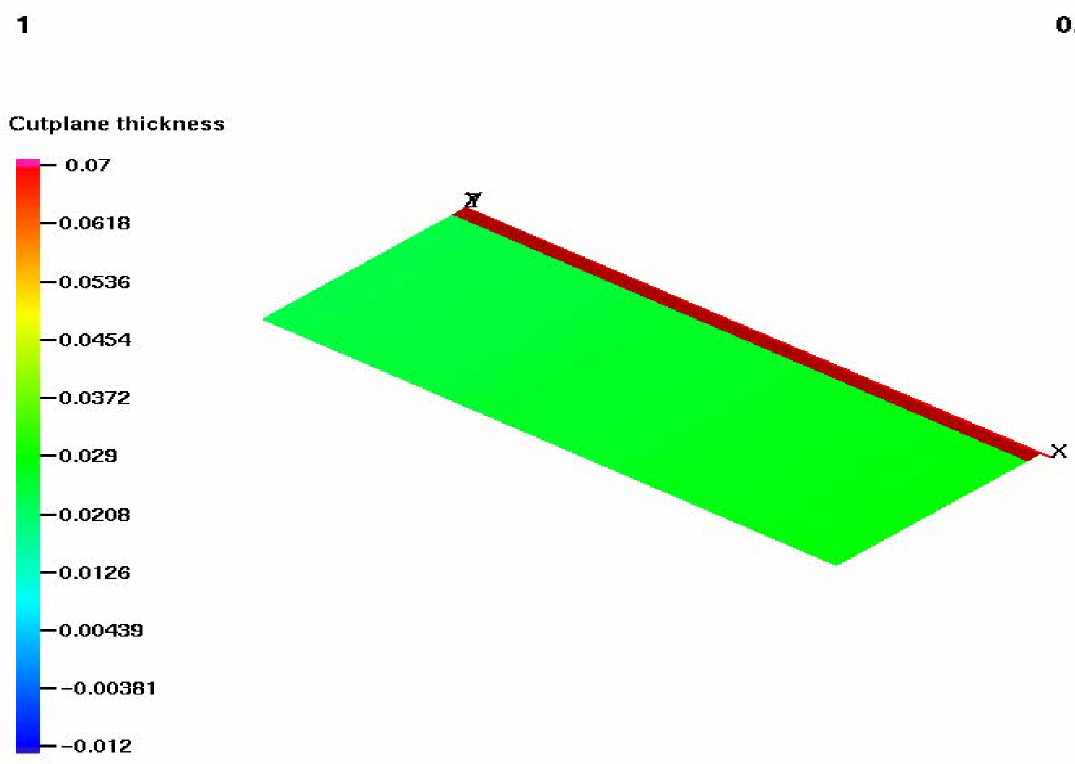


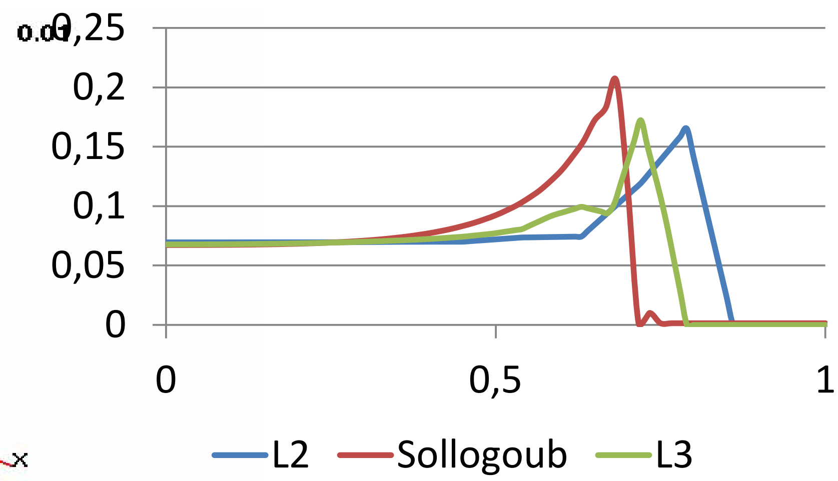


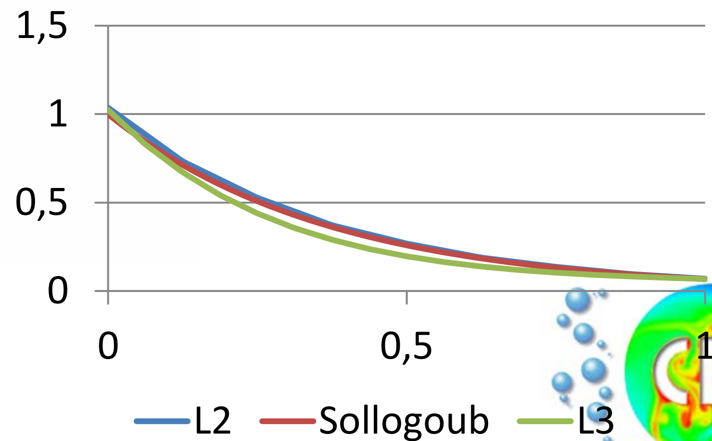
Source: Schöppner, Wibbeke 2012

Polymer stretching:

- A 2D+1 membrane model from Sollogoub et. al







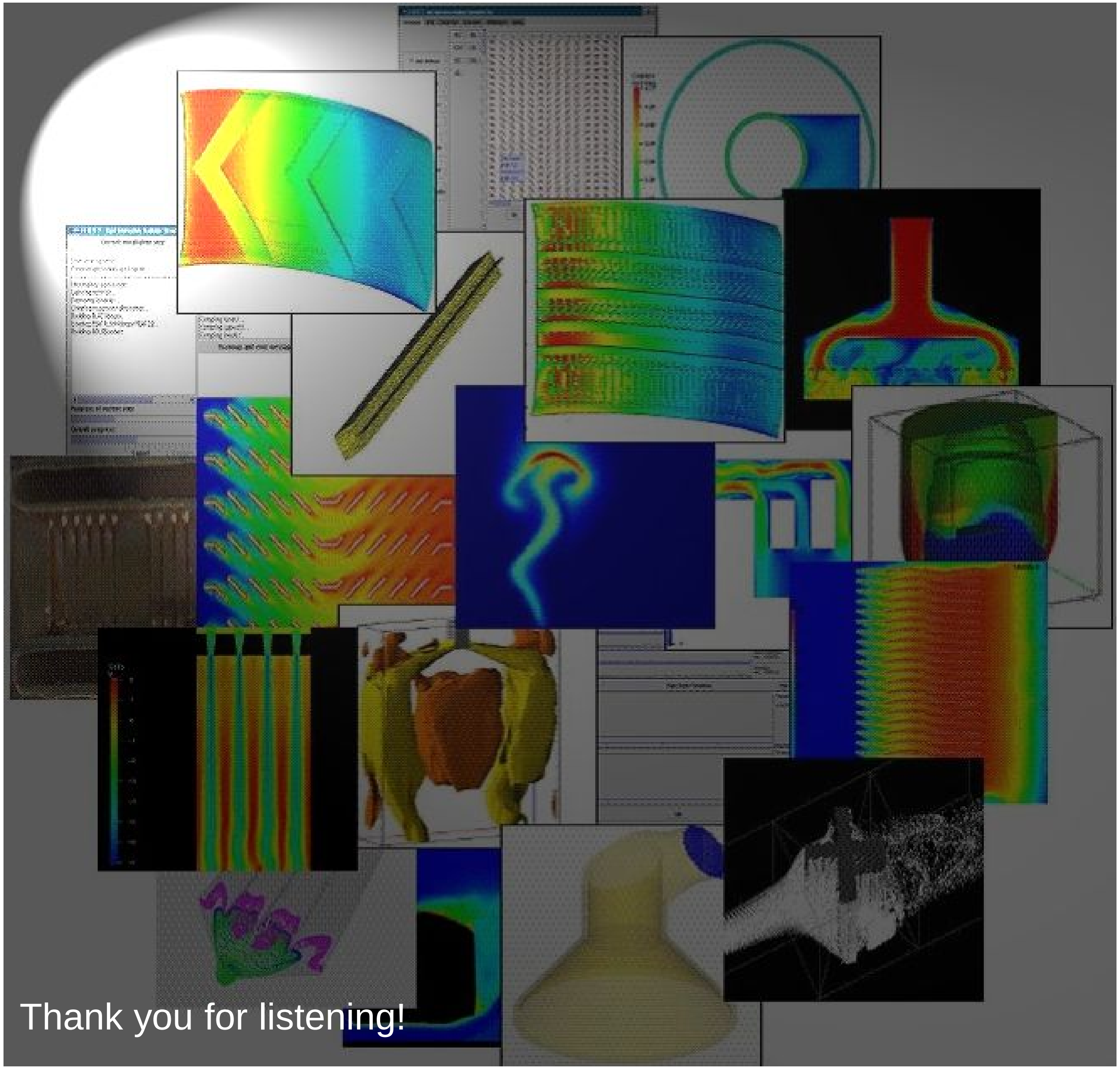
Conclusion

We have presented:

- LCR-based viscoelastic models
- Higher order FEM discretizations
- Black-box Newton-multigrid solver
- Numerical examples:
  - 2D benchmark flow around cylinder
  - Rising bubble surrounded by viscoelastic fluid
  - 3D solver for LCR-based viscoelastic models
  - Polymer stretching

We would like in the future:

- 3D viscoelatic multiphase
- Collection of different viscoelastic models
- FBM and viscoelastic integral model


Thank you for listening!