Monolithic Newton multigrid FEM techniques for nonlinear problems with special emphasis on viscoelastic fluids

H. Damanik, J. Hron, A. Ouazzi, S. Turek

Institut für Angewandte Mathematik, LS III, TU Dortmund

http://www.mathematik.tu-dortmund.de/lsiii

ENUMATH 2011, September 5 – 9, 2011
University of Leicester,
Leicester, UK

Governing equations

- **Generalized Navier-Stokes equations**

$$\rho\left(\frac{\partial}{\partial t}+u\cdot\nabla\right)u = -\nabla p + \nabla\cdot\sigma, \quad \nabla\cdot u = 0,$$

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

$$D(u)=\frac{1}{2}\left(\nabla u+(\nabla u)^T\right),$$

$$\sigma = \sigma_s + \sigma_p .$$

- **Viscous stress**

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

- **Elastic stress**

$$\sigma_p + We\frac{\delta_a\sigma_p}{\delta t} + G(\sigma_p, D) + H(\sigma_p) = 2\eta_p D(u).$$

Constitutive Models (I)

technische universität dortmund

- **Viscous stress**

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

- **Power law model**

$$\eta_s(\dot\gamma,\Theta,p) = \eta_0(\varepsilon + \dot\gamma^2)^{(\frac{r}{2}-1)},(\eta_0 > 0, r > 1).$$

- **Generalized Cross model**

$$\eta_s(\dot\gamma,\Theta,p) = \eta_\infty + \frac{(\eta_0 - \eta_\infty)}{(1+(\lambda\dot\gamma)^{r_1})^r}\exp(\alpha p + (a_1 + \frac{a_2}{a_3+\Theta})),$$

$$(\eta_0 > \eta_\infty \geq 0, r > 1, \lambda > 0).$$

- **Elastic stress**

$$\sigma_p + We\frac{\delta_a \sigma_p}{\delta t} + G(\sigma_p, D) + H(\sigma_p) = 2\eta_p D(u).$$

- **Upper/Lower convective derivative**

$$\frac{\delta_a \sigma}{\delta t} = \left(\frac{\partial}{\partial t} + u \cdot \nabla\right)\sigma + g_a(\sigma, \nabla u)$$

$$\begin{aligned} g_a(\sigma,\nabla u) &= \frac{1-a}{2}\left(\sigma \nabla u + (\nabla u)^T \sigma\right) \\ &- \frac{1+a}{2}\left(\nabla u \sigma + \sigma(\nabla u)^T\right), \quad a = \pm 1 \end{aligned}$$

- **Generalized differential constitutive model**

$$\sigma_p + We\frac{\delta_a \sigma_p}{\delta t} + G(\sigma_p,\ D) + H(\sigma_p) = 2\eta_{\mathrm{p}} D(u).$$

- **Oldroyd-B** $G = 0,\ H = 0,\ a = 1.$

- **Giesekus** $G = 0,\ H = \alpha\sigma_p^2,\ a = 1.$

- **Phan-Thien and Tanner**

$$G = 0, \quad H = \left[\exp(\alpha\, tr(\sigma_p)) - 1\right]\sigma_p\,.$$

- **White and Metzner**

$$G = \alpha(2D : D)^{\frac{1}{2}}, \quad H = 0.$$

Numerical Challenges

technische universität dortmund

- **FEM techniques have to handle the following challenges points**

  - **Stable FE spaces for velocity/pressure and velocity/stress interpolation** $Q_2/Q_2/P_1^{disc}$ **or** $\tilde{Q}_1/\tilde{Q}_1/P_0$ **or the new** $\tilde{Q}_2/\tilde{Q}_2/P_1^{disc}$
  - **Special treatment of the convective terms: edge-oriented/interior penalty (EO-FEM), TVD/FCT**
  - **High Weissenberg number problem (HWNP): LCR**

- **Solvers have to deal with different sources of nonlinearity**

  - **Nonlinearity: Newton method**
  - **Strong coupling of equations: monolithic multigrid approach**

- **Complex geometries (and meshes)**

Old → (u, p, σ_p)

$$\left.\begin{aligned}&\rho\left(\frac{\partial}{\partial t}+u\cdot\nabla\right)u=-\nabla p+2\nabla\cdot\eta_s D+\nabla\cdot\sigma_p,\ \nabla\cdot u=0,\\&\sigma_p+We\frac{\delta_a\sigma_p}{\delta t}=2\eta_p D,\end{aligned}\right\}\quad(1)$$

Conformation tensor → (u, p, σ_c) This tensor is positive definite by design !!

Replace σ_p in (1) with $\sigma_p=\frac{\eta_p}{We}(\sigma_c-\mathrm{I})$ → special discretization : TVD

$$\left.\begin{aligned}&\rho\left(\frac{\partial}{\partial t}+\mathrm{u}\cdot\nabla\right)u=-\nabla p+2\nabla\cdot\eta_s D+\frac{1}{We}\nabla\cdot\eta_p\sigma_c,\ \nabla\cdot\mathrm{u}=0,\\&\frac{\delta_a\sigma_c}{\delta t}+\frac{1}{We}(\sigma_c-\mathrm{I})=0,\end{aligned}\right\}\quad(2)$$

Conformation Tensor Properties

$$\sigma_c(t) = \int_{\infty}^{t} \frac{1}{\mathrm{We}^2} \exp\left(\frac{-(t-s)}{\mathrm{We}}\right) F(s,t)\, F(s,t)^T\, ds$$

Positive by design,
so we can take its logarithm

<u>2 Observations:</u>

- positive definite → special discretizations like FCT/TVD
- exponential behaviour → approximation by polynomials???

Problem Reformulation (II)

Replace σ_c in (2) with $\sigma_c = e^{\sigma_{lc}}$

$$\left.\begin{aligned} &\rho\left(\frac{\partial}{\partial t} + u \cdot \nabla\right)u = -\nabla p + 2\nabla \cdot \eta_s D + \frac{1}{\mathrm{We}} \nabla \cdot \eta_p e^{\sigma_{lc}}, \ \nabla \cdot u = 0, \\ &\frac{\delta_a e^{\sigma_{lc}}}{\delta t} + \frac{1}{We}\left(e^{\sigma_{lc}} - \mathrm{I}\right) = 0, \end{aligned}\right\} \quad \textbf{(3)}$$

Gradient of exponential of $e^{\sigma_{lc}}$ → ???

Solvers → ???

LCR Formulation

- **Experience:**
  - **Stresses grow exponentially**
  - **Conformation tensor is positive by design**

- **Idea**
  - **Take the logarithm as a new variable** $\sigma_{lc} = \log \sigma_c$ **using the eigenvalue decomposition**

$$\sigma_{lc} = R \log(\lambda_{\sigma_c}) R^T$$

  - **Decompose the velocity gradient inside the stretching part**

$$\nabla u = \Xi + \Upsilon + \overline{\Xi} \tau^{-1}$$

$$\nabla_{\sigma_c} u = R^T (\nabla u) R, \Upsilon(\nabla_{\sigma_c} u) = R\left[diag(\nabla_{\sigma_c} u))\right]R^T, \; \Xi = R[\omega \chi]R^T, \; \overline{\Xi} = R[\overline{\omega} \chi]R^T, \; \chi = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

$$\omega = \lambda_2 [\nabla_{\sigma_c} u]_{12} + \lambda_1 [\nabla_{\sigma_c} u]_{21} / (\lambda_2 - \lambda_1), \overline{\omega} = [\nabla_{\sigma_c} u]_{21} + [\nabla_{\sigma_c} u]_{21} / (\lambda_2^{-1} - \lambda_1^{-1}).$$

Full Set of Equations (LCR)

- **Generalized Newtonian (VP)**

$$\rho\left(\frac{\partial}{\partial t}+u\cdot\nabla\right)u=-\nabla p+\nabla\cdot\big(2\eta_s(\dot{\gamma},\Theta,p)D(u)\big)+\frac{1}{We}\nabla\cdot\eta_p e^{\sigma_{lc}},\quad \nabla\cdot u=0,$$

- **Non-isothermal effect (T)**

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

- **Stress equation (S)**

$$\left(\frac{\partial}{\partial t}+u\cdot\nabla\right)\sigma_{lc}-(\Xi\,\sigma_{lc}-\sigma_{lc}\,\Xi)-2\Upsilon=\frac{1}{We}f(\sigma_{lc}).$$

  - **Oldroyd-B model** $$f(\sigma_{lc})=\left(e^{-\sigma_{lc}}-I\right).$$

  - **Giesekus model** $$f(\sigma_{lc})=\left(e^{-\sigma_{lc}}-I\right)-\alpha e^{\sigma_{lc}}\left(e^{-\sigma_{lc}}-I\right)^2.$$

FEM Discretization

- **High order $Q_2 / Q_2 / P_1^{disc}$ for velocity-stress-pressure**
  - **Advantages:**
    - **Inf-sup stable for velocity and pressure**
    - **High order: good for accuracy**
    - **Discontinuous pressure: good for solver**
  - **Disadvantages:**
    - **Stabilization for same spaces for stress-velocity**
    - **a single d.o.f. belongs to four elements (in 2D)**

Compatibility condition between the stress and velocity spaces via EO-FEM !

EO-FEM

- **Edge-oriented stabilization for**
  - **Same finite element interpolation velocity and stress**
  - **convective dominated problem**

$$\langle J_{\tilde{u}}\tilde{u},\tilde{v}\rangle = \sum_{edgeE} \max\left(\gamma_u \eta_p h_E, \gamma_{\tilde{u}} h_E^2\right)\int_E [\nabla\tilde{u}][\nabla\tilde{v}]ds$$

with $\tilde{u} = (u,\sigma,\Theta)$, $\tilde{v} = (v,\tau,\Phi)$ **and** $[\nabla\tilde{u}][\nabla\tilde{v}] = \sum_i [\nabla\tilde{u}_i][\nabla\tilde{v}_i]$

Efficient Newton-type and multigrid solvers can be easily applied !

- **Damped Newton results in the solution of the form**

$$R(x) = 0, \quad x = (u, \sigma, \Theta, p)$$

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

- **Inexact Newton:** Jacobian is approximated using finite differences

$$\left[\frac{\partial R(x^{l})}{\partial x} \right]_{ij} \approx \frac{R_j(x + \varepsilon e_i) - R_j(x - \varepsilon e_i)}{2\varepsilon}$$

Jacobian matrix

- **The Jacobian matrix takes the form**

$$\left[\frac{\partial R(x^n)}{\partial x}\right] = \begin{bmatrix} A & \tilde{B}^T \\ B & 0 \end{bmatrix}$$

- **Generalized non-isothermal non-Newtonian problem**

$$A = \begin{bmatrix} A_u & \tilde{C}^T & \tilde{H}^T \\ C & A_\sigma & 0 \\ H & 0 & A_\Theta \end{bmatrix}$$

Typical saddle point problem !

Linear Solver

- **Monolithic multigrid solver**

  - **Standard geometric multigrid approach**

  - **Full** Q_2, P_1^{disc} **restrictions and prolongations**

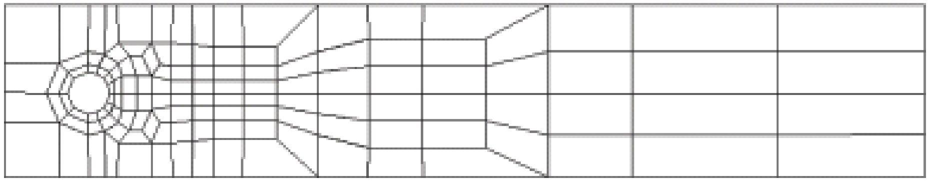
  - **Local MPSC via Vanka-like smoother**

$$\begin{bmatrix}\tilde{u}^{l+1}\\ p^{l+1}\end{bmatrix} = \begin{bmatrix}\tilde{u}^{l}\\ p^{l}\end{bmatrix} + \omega^{l} \sum_{T\in T_h} \left[\mathrm{A}_{|T}\right]^{-1} \begin{bmatrix} R_u(\tilde{u}^{l}, p^{l})\\ R_p(\tilde{u}^{l}, p^{l})\end{bmatrix}_{|T}$$

Fully implicit Monolithic FEM-Multigrid Solver !

Problem Informations

- Croarse grid and mesh information

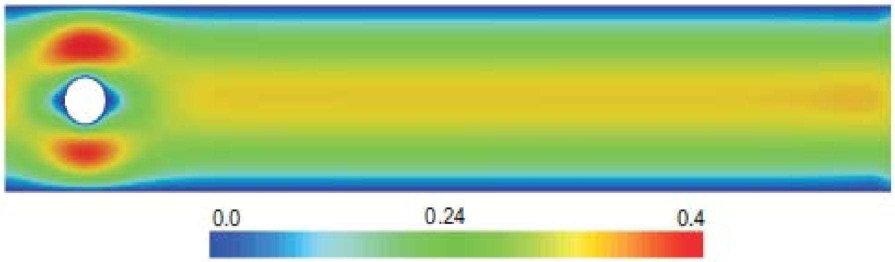


Level	NEL	NMT	NMP
1	520	572	1092
2	2080	2184	4264
3	8320	8528	16848
4	33280	33696	66976
5	133120	133952	267072

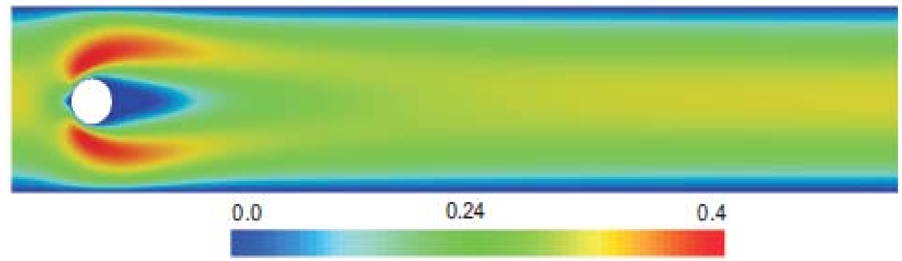
- n.o.f. for different problems

Level	n.o.f. u	n.o.f p	n.o.f. T	n.o.f S	VP	VPT	VSP
0	1144	390	572	1716	1534	2106	3250
1	4368	1560	2184	6552	5928	8112	12489
2	17056	6240	8528	25584	23296	31824	48880
3	67392	24960	33696	101088	92352	126048	193449
4	267904	99840	133952	401856	367744	501696	769600
5	1068288	399360	534144	1602432	1467648	2001792	3070080

Stokes



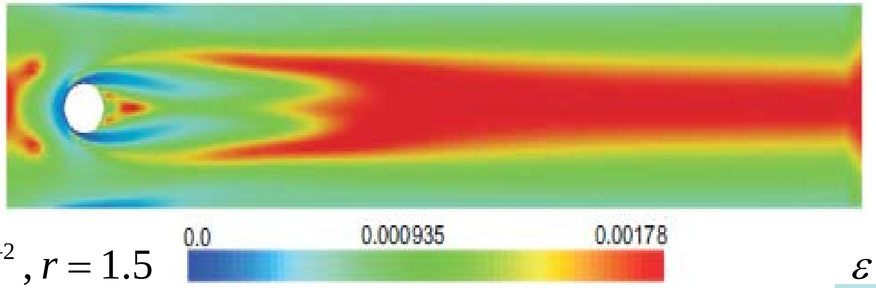
Navier-Stokes Re=20



Level	Drag	Lift	N/L	Drag	Lift	N/L
1	3.112646	2.965870e-2	1/6	5.540999	9.447473e-3	5/2
2	3.134342	3.005275e-2	1/7	5.566928	1.046885e-2	5/2
3	3.140327	3.015909e-2	1/7	5.576088	1.056787e-2	5/2
4	3.141893	3.018665e-2	1/7	5.578652	1.060398e-2	5/2
5	3.142292	3.019366e-2	1/7	5.579313	1.061503e-2	5/2

Level independent solver !

Power law problem (VP)



$$\eta_s(\dot{\gamma},\Theta,p)=\eta_0(\varepsilon+\dot{\gamma}^2)^{(\frac{r}{2}-1)},(\eta_0>0,r>1).$$

$\varepsilon=10^{-2}, r=1.5$

Level	Drag	Lift	N/L
2	3.26420	-0.01339	4/2
3	3.27728	-0.01341	3/2
4	3.27956	-0.01338	2/2
5	3.28007	-0.01337	2/2

$\varepsilon=10^{-4}, r=1.5$

Level	Drag	Lift	N/L
2	3.26433	-0.01342	4/2
3	3.27739	-0.01342	3/2
4	3.27968	-0.01339	2/2
5	3.28019	-0.01338	2/2

$\varepsilon=10^{-2}, r=3$

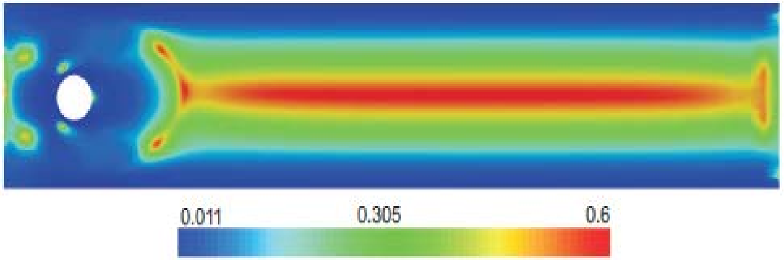
Level	Drag	Lift	N/L
2	13.74280	0.35070	3/2
3	13.77355	0.34963	3/2
4	13.78220	0.35062	3/1
5	13.78445	0.35112	2/2

$\varepsilon=10^{-4}, r=3$

Level	Drag	Lift	N/L
2	13.73800	0.35052	3/2
3	13.76875	0.34941	3/2
4	13.77740	0.35040	3/1
5	13.77970	0.35091	2/2

Level and parameter independent solver !

Cross model problem (VP)



$$\eta_s(\dot{\gamma},\Theta,p)=\eta_\infty+\frac{(\eta_0-\eta_\infty)}{(1+(\lambda\dot{\gamma})^{r_1})^r}\exp(\alpha\,p+(a_1+\frac{a_2}{a_3+\Theta})),$$

$$\eta_\infty=10^{-3},\,a_1=a_2=0,$$

$r=1, r_1=1, \alpha=0, \eta_0=10^{-2}$

Level	Drag	Lift	N/L
2	6.31313	0.02478	3/1
3	6.32337	0.02504	3/2
4	6.32619	0.02509	3/2
5	6.32691	0.02510	2/2

$r=0, r_1=1, \alpha=0.1, \eta_0=10^{-1}$

Level	Drag	Lift	N/L
2	534.29750	6.53247	3/2
3	535.48500	6.55813	3/3
4	535.77950	6.56464	3/3
5	535.84800	6.56621	2/2

$r=0\; r_1=1, \alpha=0.1, \eta_0=10^{-2}$

Level	Drag	Lift	N/L
2	33.22763	0.81901	2/2
3	33.29026	0.82140	2/2
4	33.30657	0.82201	2/2
5	33.31069	0.82217	2/2

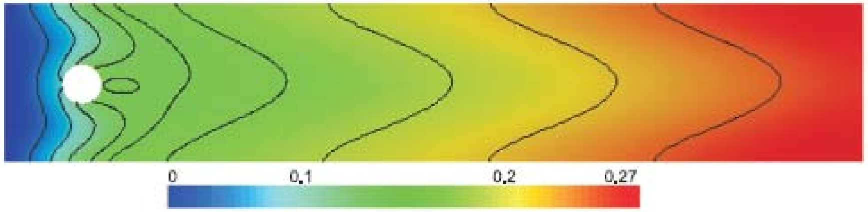
$r=1, r_1=1, \alpha=0.1, \eta_0=10^{-1}$

Level	Drag	Lift	N/L
2	15.16395	0.13886	4/3
3	15.18516	0.13963	4/3
4	15.19108	0.13978	4/3
5	15.19262	0.13982	3/3

Level and model independent solver !

Cross model problem (VTP)

Non heated cylinder



$$\eta_s(\dot{\gamma},\Theta,p) = \eta_\infty + \frac{(\eta_0 - \eta_\infty)}{(1+(\lambda\dot{\gamma})^{r_1})^{r}} \exp(\alpha\, p + (a_1 + \frac{a_2}{a_3+\Theta})),$$

$$\eta_\infty = 10^{-3}, a_1 = 0, a_3 = 1, k_1 = k_2 = 10^{-2},$$

$r = 0, r_1 = 1,\ \alpha = 0, \eta_0 = 10^{-2}, a_2 = 0.$

Level	Drag	Lift	N/L
2	74.29465	1.31636	2/2
3	74.43290	1.32009	2/2
4	74.46910	1.32105	2/2
5	74.47830	1.32129	2/2

$r = 0.1, r_1 = 1,\ \alpha = 0, \eta_0 = 10^{-1}, a_2 = 0.$

Level	Drag	Lift	N/L
2	5579.355	54.79350	3/2
3	5589.415	54.96815	3/3
4	5592.050	55.01415	3/3
5	5592.725	55.02585	3/2

$r = 0.1, r_1 = 1,\ \alpha = 0, \eta_0 = 10^{-2}, a_2 = 1.$

Level	Drag	Lift	N/L
2	53.78930	1.05488	2/2
3	53.88590	1.05770	3/2
4	53.91125	1.05844	2/2
5	53.91770	1.05863	2/2

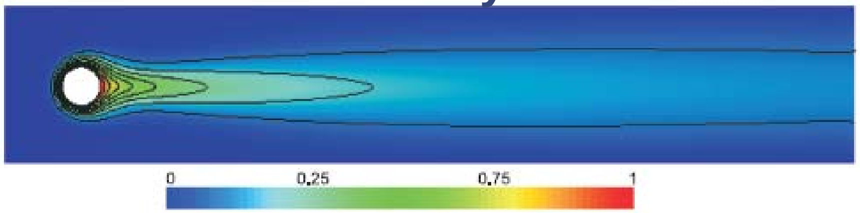
$r = 0.1, r_1 = 1,\ \alpha = 10^{-3}, \eta_0 = 10^{-1}, a_2 = 1.$

Level	Drag	Lift	N/L
2	6005.265	59.75125	3/2
3	6016.220	59.94455	3/2
4	6019.075	59.99535	3/2
5	6019.795	60.00820	3/2

Level and model independent solver !

Cross model problem (VTP)

Heated cylinder



$$\eta_s(\dot{\gamma},\Theta,p)=\eta_\infty+\frac{(\eta_0-\eta_\infty)}{(1+(\lambda\dot{\gamma})^{r_1})^r}\exp(\alpha\, p+(a_1+\frac{a_2}{a_3+\Theta})),$$

$$\eta_\infty=10^{-3}, r=0.1, r_1=1, \alpha=10^{-3}, a_1=0, a_2=1, a_3=1,$$

$\eta_0=10^{-2}, k_1=k_2=10^{-2}.$

Level	Drag	Lift	N/L
2	45.26969	0.90303	3/2
3	45.35251	0.90563	3/2
4	45.37431	0.90632	2/2
5	45.37988	0.90649	2/2

$\eta_0=10^{-1}, k_1=k_2=10^{-3}.$

Level	Drag	Lift	N/L
2	512.7765	5.37640	3/2
3	513.7120	5.39301	3/3
4	513.9585	5.39743	3/3
5	514.0215	5.39856	3/2

$\eta_0=10^{-1}, k_1=k_2=10^{-2}.$

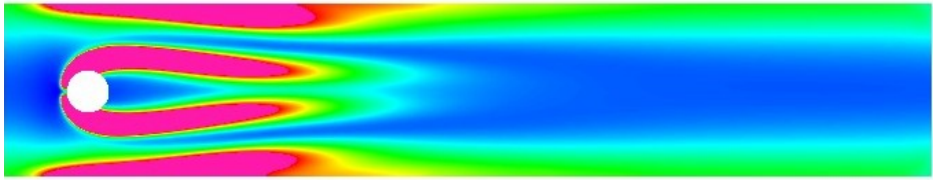
Level	Drag	Lift	N/L
2	464.07865	4.90752	2/2
3	464.93045	4.92313	3/2
4	465.15470	4.92724	2/2
5	465.21195	4.92828	2/2

$\eta_0=1.0, k_1=k_2=10^{-3}.$

Level	Drag	Lift	N/L
2	5528.860	53.11685	3/2
3	5539.025	53.28790	3/2
4	5541.690	53.33335	3/2
5	5542.365	53.34490	3/2

Level and model independent solver !

Viscoelastic fluids (VSP)



$$\sigma_p + We\frac{\delta_a \sigma_p}{\delta t} + G(\sigma_p, D) + H(\sigma_p) = 2\eta_p D(u)$$

$We = 0.002$ $a = 1, G = 0, H = 0$

Level	Drag	Lift	N/L
2	5.57150	0.01031	2/2
3	5.58032	0.01047	3/2
4	5.58285	0.01051	2/2
5	5.58351	0.01052	2/2

$We = 1.0$ $a = 1, G = 0, H = 0$

Level	Drag	Lift	N/L
2	20.8412	0.32761	7/7
3	17.7123	0.22910	6/8
4	15.0096	0.14311	6/9
5	12.58895	0.07002	6/9

$We = 0.002$ $a = 1, G = 0, H = \alpha\sigma_p^2$

Level	Drag	Lift	N/L
2	5.56474	0.01053	2/2
3	5.57511	0.01064	2/2
4	5.57936	0.01062	2/2
5	5.58131	0.01059	2/2

$We = 1.0$ $a = 1, G = 0, H = \alpha\sigma_p^2$

Level	Drag	Lift	N/L
2	5.03961	-0.00172	4/2
3	4.93834	-0.00210	4/3
4	4.84483	-0.00252	3/3
5	4.77541	-0.00276	3/4

Level independent solver !

Summary

Robust numerical and algorithmic tools are available using

- ✓ **Monolithic Finite Element Method (M-FEM)**
- ✓ **Classical and Log Conformation Reformulation (LCR)**
- ✓ **Edge Oriented stabilization (EO-FEM)**
- ✓ **Fast Newton-Multigrid Solver with local MPSC smoother**

for the simulation of nonlinear flow with viscoelastic behaviour

Advantages

- ✓ **No CFL-condition restriction due to the fully implicit coupling**
- ✓ **Positivity preserving**
- ✓ **Higher order and local adaptivity**