Cracking the high-Weissenberg number problem

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Observation (last 25 years): All numerical methods break down when the Weissenberg number exceeds a critical value. The precise critical value varies with the viscoelastic model, numerical method and mesh used.

⇒ High Weissenberg number problem (HWNP).

▷ It is believed to have a numerical origin.

▷ It is still there, despite:

– realistic constitutive models (pom-pom, XPP, FENE, . . . )
– advances in ‘stable’ computational methods (DEVSS, SUPG, DG, . . . )
Introduction (HWNP) (2)

For example:

Oldroyd-B: break down at $Wi = 0.88$

Giesekus: break down at $Wi = 1.2$
The situation is quite different than classical CFD at large Reynolds numbers, where:

- stable calculations can be performed, but

- accuracy is lost due to insufficient mesh resolution.

Research efforts are directed towards fast and accurate numerical schemes on big computers to solve problems for a better understanding of basic phenomena, such turbulence.

⇒ The situation in Computational Rheology seems hopeless . . .
Introduction (HWNP) (4)

... until a couple of months ago, that is:


where:

- the mechanism for the HWNP has been identified

- a solution has been proposed

This talk: a more ‘mechanical’ derivation, application to FEM, convince you that the HWNP has been solved and what’s left to do!
Basic equations

Momentum balance and mass balance:

\[ \nabla p - \nabla \cdot (2\eta_s D) - \nabla \cdot \tau = 0 \]
\[ \nabla \cdot u = 0 \]

with \( D = \frac{1}{2}(L + L^T) \) and \( L = (\nabla u)^T \).

Constitutive equation:

\[ \dot{c} = L \cdot c + c \cdot L^T + f(c), \quad \tau = \frac{\eta}{\lambda} (c - I) \]

with

\[ f(c) = \begin{cases} 
\frac{1}{\lambda} (c - I) & \text{Oldroyd-B} \\
\frac{1}{\lambda} (c - I + \alpha (c - I)^2) & \text{Giesekus}
\end{cases} \]
Numerical methods

Eulerian setting: \( \dot{c} = \frac{\partial c}{\partial t} + u \cdot \nabla c \)

FEM: quads with \( u \in (Q_2)^2, p \in P_1^d \)
DEVSS: projected \( D \in (P^1)^3 \)
DG: \( c \in (Q_1)^3 \)

Explicit time integration: Euler forward (1\textsuperscript{st} order) or Adams-Bashforth (2\textsuperscript{nd} order).
Analysis of the HWNP in 1D: a numerical instability (1)

Toy problem: find \( c(x, t) \) such that

\[
\frac{\partial c}{\partial t} + a \frac{\partial c}{\partial x} = bc, \quad x \in (0, L), \quad t \geq 0
\]

with

▷ \( a > 0, \ b > 0 \)

▷ \( c(x = 0, t) = c(x, t = 0) = 1 \)

\( \Rightarrow \) exponential growth balanced by convection
Analysis of the HWNP in 1D: a numerical instability (2)

Numerical discretization in space (first-order upwind):

\[
\frac{dc_i}{dt} = -a \frac{c_i - c_{i-1}}{\Delta x} + bc_i
\]

or in matrix form

\[
\frac{dc}{dt} = Ac
\]

with

\[
A = \begin{pmatrix} \gamma & \gamma & 0 \\ \beta & \gamma & \ldots \\ 0 & \ldots & \beta & \gamma \end{pmatrix}, \quad \gamma = b - \frac{a}{\Delta x}, \quad \beta = \frac{a}{\Delta x}
Analysis of the HWNP in 1D: a numerical instability (3)

To avoid exponential growth in time:

\[ \gamma = b - \frac{a}{\Delta x} \leq 0 \quad \text{or} \quad \Delta x \leq \frac{a}{b} \]

Define \( C \):

\[ C = \frac{\Delta x b}{a}, \quad \text{or for } a, b \in \mathbb{R} : \quad C = \frac{\Delta x \max(b, 0)}{|a|} \]

then for stability:

\[ C \leq 1 \quad \text{first-order upwind} \]

For DG using linear polynomials:

\[ C \leq 2 \quad \text{DG with } P_1 \]

\[ \Rightarrow \text{Failure to balance exponential growth with convection when criterion violated.} \]
Analysis of the HWNP in 1D: a numerical instability (4)

For Oldroyd-B in extension: \( a = u, \ b = 2\dot{\epsilon} - \frac{1}{\lambda}, \) with \( \dot{\epsilon} = \frac{\partial u}{\partial x} : 

\[ C = \frac{\Delta x \max(2\dot{\epsilon} - \frac{1}{\lambda}, 0)}{|u|} \]

For Giesekus in extension: \( a = u, \ b = 2\dot{\epsilon} - \frac{1}{\lambda}(1 + 2\alpha c_{xx}), \)

\[ C = \frac{\Delta x \max(2\dot{\epsilon} - \frac{1}{\lambda}(1 + 2\alpha c_{xx}), 0)}{|u|} \]
Solution to the problem: log transformation

Solution: solve for \( s = \log c \).

PDE for \( s \):

\[
\dot{s} = \frac{\dot{c}}{c} = \frac{bc}{c} = b
\]

with \( \dot{s} = \frac{\partial s}{\partial t} + a \frac{\partial s}{\partial x} \), and thus:

\[
\frac{\partial s}{\partial t} + a \frac{\partial s}{\partial x} = b, \quad x \in (0, L), \quad t \geq 0
\]

and \( c = \exp(s) \).

\( \Rightarrow \) No numerical instability. No restrictions on \( \Delta x \)
Log transformation for tensors

$\log \tau_{ij}$: No

$\log \tau$: No

$\log c_{ij}$: No

$\log c$: YES!

Thus we choose $s = \log c$.

**BONUS:** $c = \exp(s)$ *always positive definite!*. 
Evolution equation for \( s = \log c \) \hspace{1cm} (1)

Spectral decomposition:

\[
c = c_1 n_1 n_1 + c_2 n_2 n_2 + c_3 n_3 n_3 = \sum_{i=1}^{3} c_i n_i n_i,
\]

\[
c = \begin{pmatrix} c_1 & 0 & 0 \\ 0 & c_2 & 0 \\ 0 & 0 & c_3 \end{pmatrix}
\]

\[
s = \log c = \sum_{i=1}^{3} \log(c_i) n_i n_i = \sum_{i=1}^{3} s_i n_i n_i,
\]

\[
s = \begin{pmatrix} \log c_1 & 0 & 0 \\ 0 & \log c_2 & 0 \\ 0 & 0 & \log c_3 \end{pmatrix} = \begin{pmatrix} s_1 & 0 & 0 \\ 0 & s_2 & 0 \\ 0 & 0 & s_3 \end{pmatrix}
\]
Evolution equation for \( s = \log c \) \hspace{1cm} (2)

Substantial derivative of \( s \):

\[
\dot{s} = \sum_{i=1}^{3} \dot{s}_i n_i n_i + \sum_{i=1}^{3} s_i \dot{n}_i n_i + \sum_{i=1}^{3} s_i n_i \dot{n}_i
\]

or with \( \dot{s}_i = \frac{d(\log c_i)}{dt} = \frac{\dot{c}_i}{c_i} \)

\[
\dot{s} = \sum_{i=1}^{3} \frac{\dot{c}_i}{c_i} n_i n_i + \sum_{i=1}^{3} s_i \dot{n}_i n_i + \sum_{i=1}^{3} s_i n_i \dot{n}_i
\]

⇒ We need expressions for \( \dot{c}_i \) and \( \dot{n}_i \)
Evolution equation for $s = \log c$ \hspace{1cm} (3)

We get $\dot{c}_i$ and $\dot{n}_i$ from the CE:

$$\dot{c} = L \cdot c + c \cdot L^T + f(c)$$

From the diagonal components (in the $n_i$-frame):

$$\dot{c}_i = 2c_i L_{ii} + f_i(c_1, c_2, c_3)$$

From the off-diagonal components (in the $n_i$-frame):

$$\dot{n}_i = \omega \cdot n_i = \sum_{j=1}^{3} \omega_{ji} n_j$$

with the components $\omega_{ij}$ of the skewsymmetric tensor $\omega$:

$$\omega_{ij} = \frac{c_i L_{ji} + c_j L_{ij}}{c_j - c_i}, \quad i \neq j, \quad c_i \neq c_j$$
Evolution equation for $s = \log c$ \hspace{1cm} (4)

End result:

$$\dot{s} = 2 \sum_{i=1}^{3} L_{ii} n_i n_i + \sum_{i=1}^{3} \frac{f_i}{c_i} n_i n_i + \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{s_i - s_j}{c_i - c_j} (c_j L_{ij} + c_i L_{ji}) n_i n_j$$

Notes:

$\triangleright \quad c_i = \exp(s_i), \quad c = \exp(s)$

$\triangleright \quad \lim_{{c_i \to c_j}} \frac{s_i - s_j}{c_i - c_j} (c_j L_{ij} + c_i L_{ji}) = L_{ij} + L_{ji} = 2D_{ij}$
Flow past a cylinder confined between two flat plates

- Oldroyd-B model with $\eta_s/\eta = 0.59$, where $\eta = \eta_s + \eta_p$
- Giesekus model with $\alpha = 0.01$.
- Weissenberg number: $Wi = \frac{\lambda U}{R}$, with $U$ average velocity in channel.
- Dimensionless drag force $K = \frac{F_x}{\eta U}$
- Dimensionless scaling: coordinates with $R$, stresses with $\frac{\eta U}{R}$, time with $R/U$, velocities with $U$.
- Periodical boundary conditions.
Mesh

M0, 120 elements

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<th>number of elements</th>
<th>M3</th>
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<th>M5</th>
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Value of $C$ on the center line in the wake for Oldroyd-B
Value of $C$ on the center line in the wake for Giesekus

![Graph showing the value of C on the center line in the wake for Giesekus with different Wi values: Wi=1.17, Wi=1.18, Wi=1.19.](image)
**Dimensionless drag coefficient \( K \) for Oldroyd-B (1)**

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Dimensionless drag coefficient $K$ for Oldroyd-B (2)
Convergence of the numerical solution for Oldroyd-B? (1)
Convergence of the numerical solution for Oldroyd-B? (2)

Wi = 1.0

\[ \text{tauxx} \]

\[ s \]

Graphs showing the convergence of numerical solutions for different models M3, M4, M5, and M4-1D, M5-1D.
Convergence of the numerical solution for Oldroyd-B? (3)

\[ s_{xx} = (\log c)_{xx} \neq \log c_{xx}! \]
Convergence of the numerical solution for Oldroyd-B? (4)

Convergence of the numerical solution for Oldroyd-B? (4)

Convergence of the numerical solution for Oldroyd-B? (4)

Convergence of the numerical solution for Oldroyd-B? (4)
Minimum value of $\det c$

$log(\det(c))$

$Wi=1.8, M4$
Giesekus with $\alpha = 0.01; \ c_{xx}$
Giesekus with $\alpha = 0.01$: convergence?

![Graph showing the behavior of Giesekus equations with Wi=5.0.](image)
Conclusions

We believe that the HWNP has been solved.

The log conformation representation is the essential part here.

We think Computational Rheology can now become a normal branch of CFD focusing on study of basic phenomena, such as flow instabilities, morphology and mixing of polymer blends, macroscopic stresses of viscoelastic particle suspensions, drag reduction at high Reynolds number flows, ... 

Remaining issues include:

- identifying model problems/artefacts
- resolution problems
- efficient schemes/solvers for large 3D problems
- ...