The High-Weissenberg Number Problem

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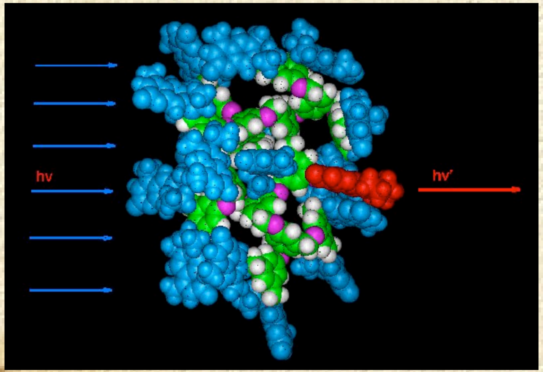
What are viscoelastic fluids?

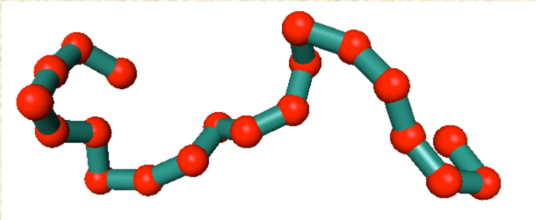
Basic facts

Viscoelastic fluids are complex fluids that have "memory" (the state-of-stress depends on the flow history)

Visco: friction, irreversibility, loss of memory
Elastic: recoil, internal energy storage

Most viscoelastic fluids are made of, or contain polymers (polymer solutions and polymer melts)

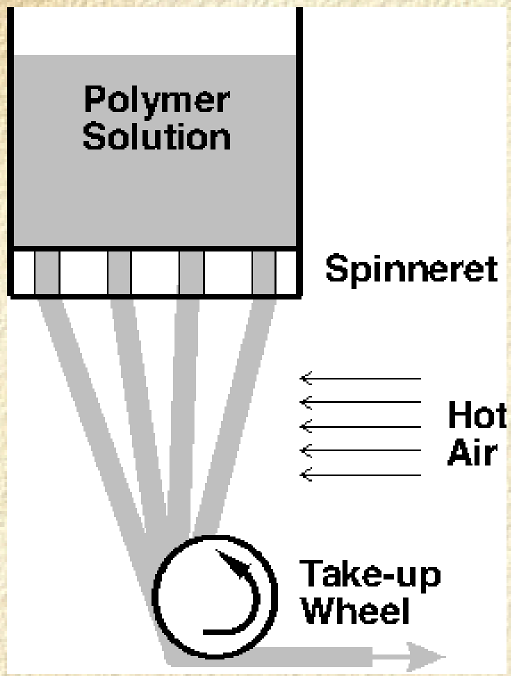




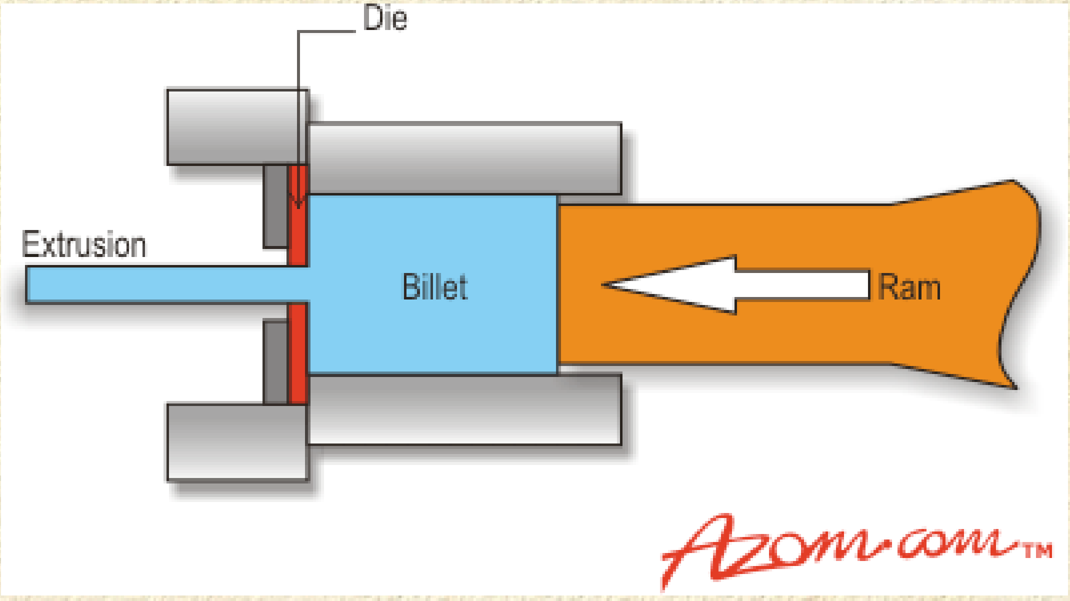
(Viscoelasticity is a matter of time scales: internal relaxation time versus macroscopic time scales)

Applications in industry

Most material processing is performed in the liquid state (molding, extrusion), and processing rates are limited by flow instabilities.



Fibre spinning



Extrusion

The fluid mechanics of complex materials is called rheology

"Peculiar" behavior of viscoelastic fluids

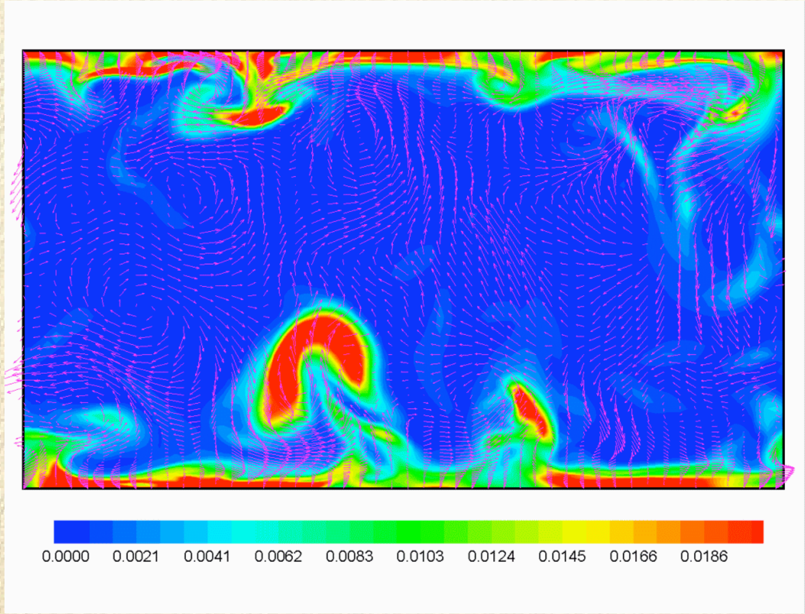
Die swell

Rod climbing

Drag reduction

Adding *a few parts per million* of polymers into a solvent can suppress turbulent flow and result in up to 80% drag reduction (first reported in 1949 by Toms).

There is no accepted model that explains this mechanism.



The modelling of polymeric fluids

From microscopic models to constitutive laws

Like all fluids, viscoelastic fluids are governed by a momentum equation:

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p + \nabla \cdot \tau$$

$\mathbf{u}(\mathbf{x}, t)$	The Eulerian velocity field
$\mathbf{p}(\mathbf{x}, t)$	The pressure field
$\tau(\mathbf{x}, t)$	The stress tensor

Viscoelastic flows are incompressible:

$$\nabla \cdot \mathbf{u} = 0$$

For Newtonian (viscous) fluids, the stress depends only on the *instantaneous* rate of deformation (Newton's law):

$$\tau = \nu(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

Substitution into the momentum equation gives the *Navier-Stokes equations:*

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p + \nu \Delta \mathbf{u}$$

For polymeric fluids there is an additional source of stress due to the polymers:

$$\tau = \nu_s(\nabla \mathbf{u} + \nabla \mathbf{u}^T) + \tau_p$$

In a viscoelastic fluid, the *extra-stress* due to polymers satisfies its own evolution equation. The relation between the extra-stress and the history of the flow is called the constitutive law of the fluid.

The modelling of constitutive laws for particular fluids is an active field of research. Many are derived from *molecular models* supplemented with *closure approximations*.

For example, stochastic model of dumbbells:

$$m\ddot{\mathbf{r}} = -k\mathbf{r} + \zeta(\dot{\mathbf{r}} - \mathbf{r} \cdot \nabla \mathbf{u}) + noise$$

$\mathbf{r}$(t) : the elongation of the polymer

$$\tau_p = nk < \mathbf{rr} >$$

By solving the corresponding Smulochowski equation one obtains the upper-convected Maxwell equation

$$\frac{\partial \tau_p}{\partial t} + (\mathbf{u} \cdot \nabla)\tau_p - (\nabla \mathbf{u})\tau_p - \tau_p(\nabla \mathbf{u})^T = -\frac{1}{\lambda}\tau_p + \frac{\nu_p}{\lambda}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

deformation

source

convection

relaxation

The model of a Newtonian stress supplemented with an extra-stress that satisfies the U.C. Maxwell equation is called the Oldroyd-B model.

$$\frac{\partial \tau_p}{\partial t} + (\mathbf{u} \cdot \nabla)\tau_p - (\nabla \mathbf{u})\tau_p - \tau_p(\nabla \mathbf{u})^T = -\frac{1}{\lambda}\tau_p + \frac{\nu_p}{\lambda}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

ν_p The polymeric viscosity

λ The relaxation time (Weissenberg number, *We*)

When *We* is small (additional) Newtonian viscosity

$$\tau_p \approx \nu_p(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

It is when *We*>1 (memory range comparable to characteristic flow time) that life becomes interesting (and complicated).

The high-Weissenberg number problem

A 30 year old mystery

Computational rheology started in the early 1970s. Mostly finite-element methods for steady 2D flows (but also some finite volumes, finite differences, spectral methods, and particle tracking methods).

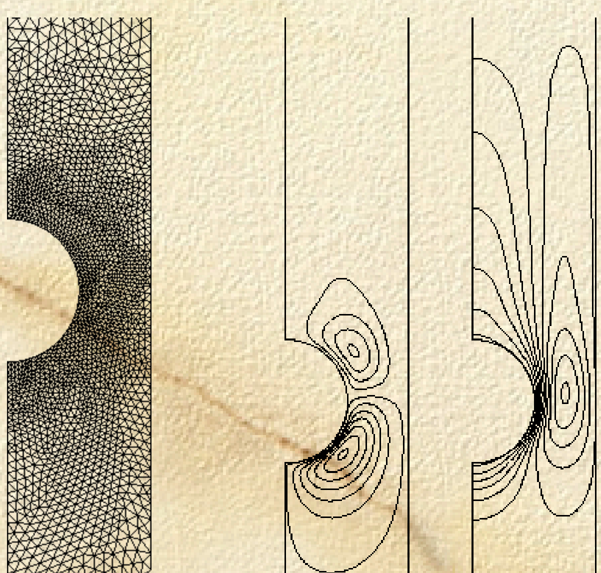
All methods, without exception, *were found to break down at a "frustratingly low value" of the Weissenberg number* (usually around We=1; precise critical value varies with the flow geometry).

The reason for this breakdown has remained somewhat of a mystery. Evidence that it is a numerical phenomenon (but inconclusive whether higher resolution delays of promotes breakdown). Yet, some still blame the invalidity of the constitutive laws.

Benchmark problem: flow through a 4:1 contraction

Breakdown for an Oldroyd-B fluid at *We* around 2.8 (Walters and Webster, 2003)

Benchmark problem: flow past a cylinder



Breakdown for an Oldroyd-B fluid at *We* around 0.9 (Fan *et al*. 1999).

The high-Weissenberg number problem has haunted computational rheology for over 30 years. It limits tremendously the application of simulations in viscoelastic material processing.

A fundamental numerical instability

A simple cartoon that explains a lot

Let's be idiots:

Take the simplest constitutive model (Oldroyd B), and your favorite numerical scheme (finite-differences, with upwinding, projection, and implicit for parabolic terms).

Above a certain *We*, the numerical solution blows up in time exponentially.

What can go wrong?

$$\frac{\partial \tau_p}{\partial t} + (\mathbf{u} \cdot \nabla)\tau_p - (\nabla \mathbf{u})\tau_p - \tau_p(\nabla \mathbf{u})^T = -\frac{1}{\lambda}\tau_p + \frac{\nu_p}{\lambda}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

convection — exponential growth

For high We and large deformation rate, the only term that can balance the exponential blowup is the convection.

This observation calls for a simple test problem:

A one-dimensional linear scalar equation with constant coefficients (is there anything simpler?)

$$\frac{\partial \phi}{\partial t} + a\,\frac{\partial \phi}{\partial x} = b\,\phi \qquad\qquad x \in [0,1]$$

$$\phi(0,t) = 1$$

The scalar field $\phi(x,t)$ moves to the right with velocity $a>0$, and is amplified at a rate $b>0$.

Steady state solution: $\phi(x) = \exp(-b\,x/a)$

Now apply any numerical method to solve this problem. For example, first-order *upwind scheme*:

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = a\frac{\phi_i^n - \phi_{i-1}^n}{\Delta x} + b\,\phi_i^n$$

which we rewrite as

$$\phi_i^{n+1} = \left(1 - \frac{a\,\Delta t}{\Delta x} + \Delta t\, b\right)\phi_i^n + \frac{a\,\Delta t}{\Delta x}\phi_{i-1}^n$$

The numerical solution blows up unless

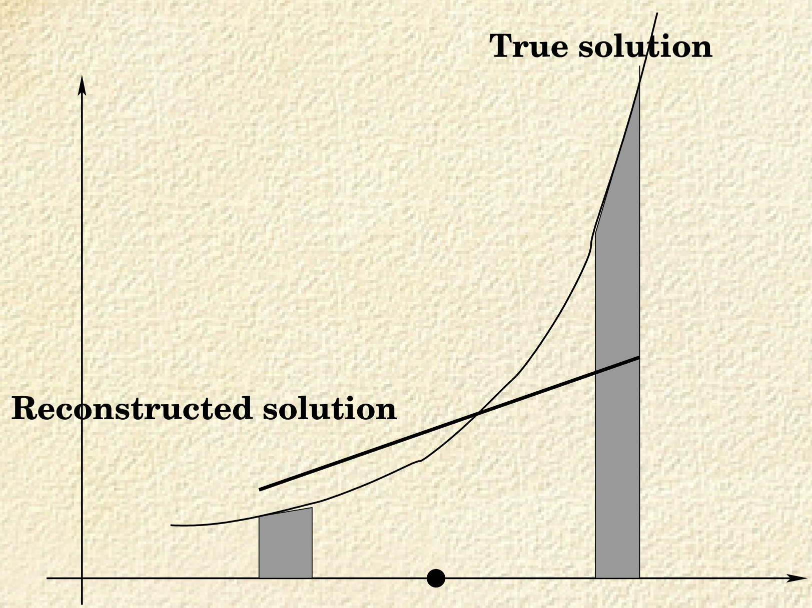
$$\boxed{\Delta x < \frac{a}{b}}$$

Restrictive when velocity is low and amplification is large

Numerics does not let you stay too long in a region of fast growth

Interpretation of the new stability condition

In a way or another all methods compute numerical fluxes



All schemes that are based on *polynomial interpolation* under-estimate the outgoing flux because *the true profile is exponential*.

The computed outgoing flux fails to balance the exponential amplification

For the U.C. Maxwell eq. the corresponding stability condition is

$$\Delta x < \frac{|\mathbf{u}|}{2\sqrt{-\det \nabla \mathbf{u}} - 1/\lambda}$$

Troubles in the vicinity of stagnation points and geometrical singularities (e.g. re-entrant corners)

The solution

Solve equations for the logarithm

Since the failure stems from bad interpolation of exponentials, let's evolve instead the logarithm!

Original equation: $$\frac{\partial \phi}{\partial t} + a \frac{\partial \phi}{\partial x} = b\,\phi$$

Transformation: $$\psi(x,t) = \log \phi(x,t)$$

Transformed equation: $$\frac{\partial \psi}{\partial t} + a \frac{\partial \psi}{\partial x} = b$$

Use your favorite scheme:

$$\psi_i^{n+1} = \left(1 - \frac{a\,\Delta t}{\Delta x}\right)\psi_i^n + \frac{a\,\Delta t}{\Delta x}\psi_{i-1}^n + \Delta t\, b$$

No restriction on Δx!!!

Cheater! you converted multiplicative growth into additive growth.

OK, then exponentiate the discrete equation for ψ, and expand exp(b Δt) ~ 1 + b Δt:

$$\phi_i^{n+1} = (\phi_i^n)^{1-a\Delta t/\Delta x}(\phi_{i-1}^n)^{a\Delta t/\Delta x} + \Delta t\, b\phi_i^n$$

Convection uses *geometric weights*

Multiplicative growth and yet *unconditionally stable*

Reformulating constitutive laws

The log-conformation representation

This little analysis suggests that we should evolve the *logarithm of the extra-stress tensor*

The stress is a second-rank tensor and therefore has a logarithm only if it is *symmetric positive-definite*

The extra-stress does not preserve positivity, but the conformation tensor

$$\sigma = \tau_p + \frac{\nu_p}{\lambda} I$$

does

The U.C. Maxwell equation in terms of the conformation tensor:

$$\frac{\partial \sigma}{\partial t} + (\mathbf{u} \cdot \nabla)\sigma - (\nabla \mathbf{u})\sigma - \sigma(\nabla \mathbf{u})^T = -\frac{1}{\lambda}(\sigma - I)$$

Goal: reformulate the constitutive law as an equation for

$$\psi(\mathbf{x}, t) = \log \sigma(\mathbf{x}, t)$$

Transformation of convection: easy! every reversible function of σ(x,t) satisfies the exact same equation.

$$\frac{\partial \sigma}{\partial t} + (\mathbf{u} \cdot \nabla)\sigma = 0 \qquad \text{implies} \qquad \frac{\partial \psi}{\partial t} + (\mathbf{u} \cdot \nabla)\psi = 0$$

Transformation of relaxation: straightforward change of variables

$$\frac{\partial \sigma}{\partial t} = -\frac{1}{\lambda}(\sigma - I) \qquad \text{implies} \qquad \frac{\partial \psi}{\partial t} = -\frac{1}{\lambda}(I - e^{-\psi})$$

Transformation of deformation: based on the following decomposition

Let σ *be a symmetric positive-definite tensor, then the velocity gradient* ∇u *has a decomposition*

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

where Ω,N *are anti-symmetric and* B *is symmetric and commutes with* σ

Decomposition of the velocity gradient into a *rotational component*, an *extensional component*, and a *"null" component*.

Constitutive law for the log-conformation

$$\frac{\partial \psi}{\partial t} + (\mathbf{u} \cdot \nabla)\psi - (\Omega\psi - \psi\Omega) - 2B = -\frac{1}{\lambda}(I - e^{-\psi})$$

rotation

(additive) extension

We claim that solving the constitutive laws using this representation (detailed scheme less important) will not exhibit a high Weissenberg number problem!

Implementation

Not so important....

The system:

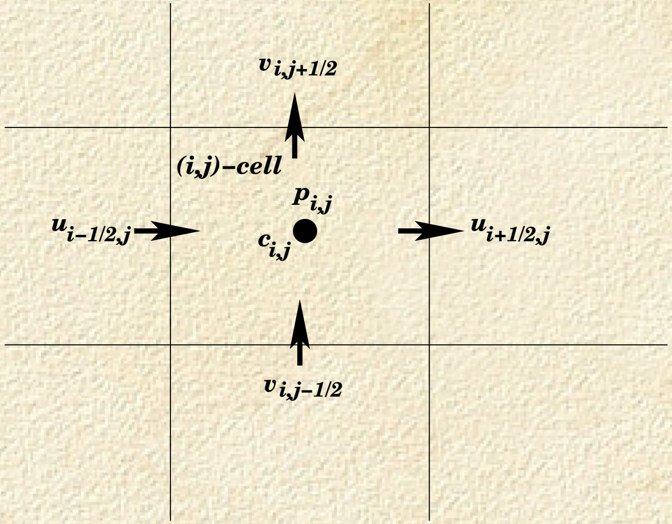
$$\frac{\partial \psi}{\partial t} + (\mathbf{u} \cdot \nabla)\psi - (\Omega\psi - \psi\Omega) - 2B = -\frac{1}{\lambda}(I - e^{-\psi})$$

$$\psi(\mathbf{x}, t) = \log \sigma(\mathbf{x}, t) \qquad \sigma = \tau_p + \frac{\nu_p}{\lambda} I$$

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p + \nabla \cdot \tau$$

Temporal discretization with a *two-step backward differentiation formula*

Spatial discretization with a *staggered grid*

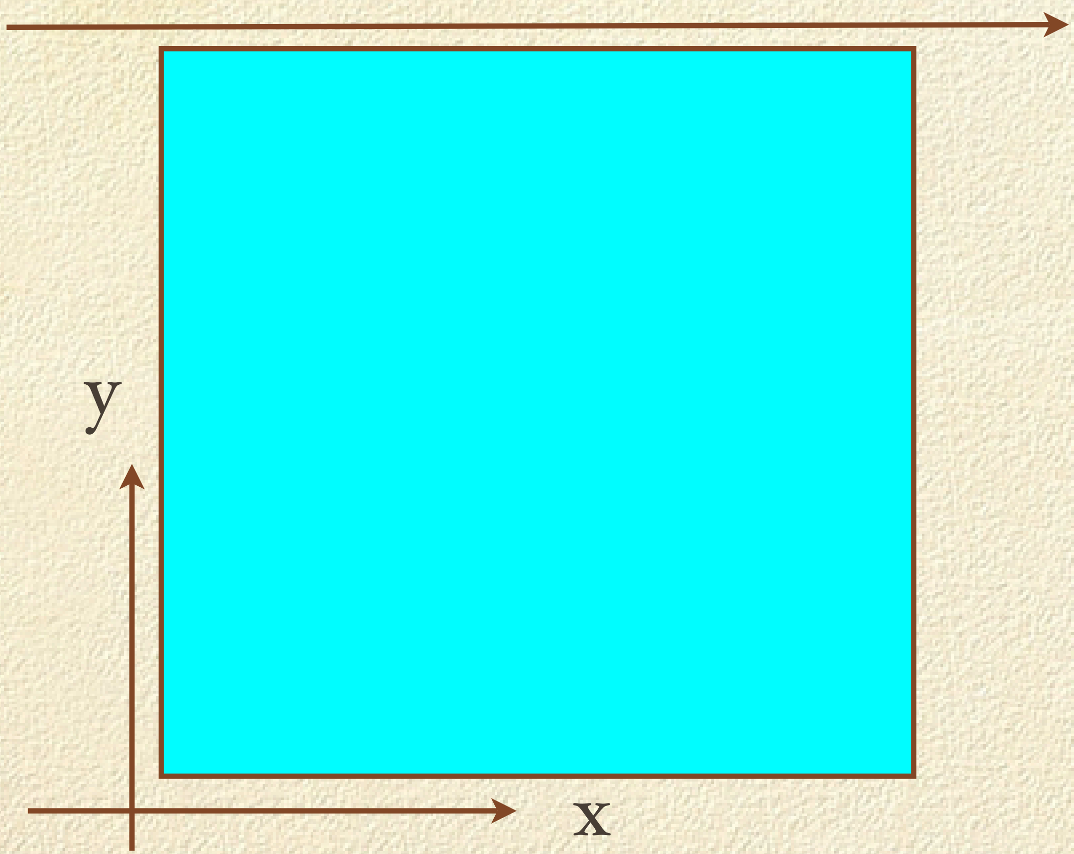


Second-order in space and time

Numerical results

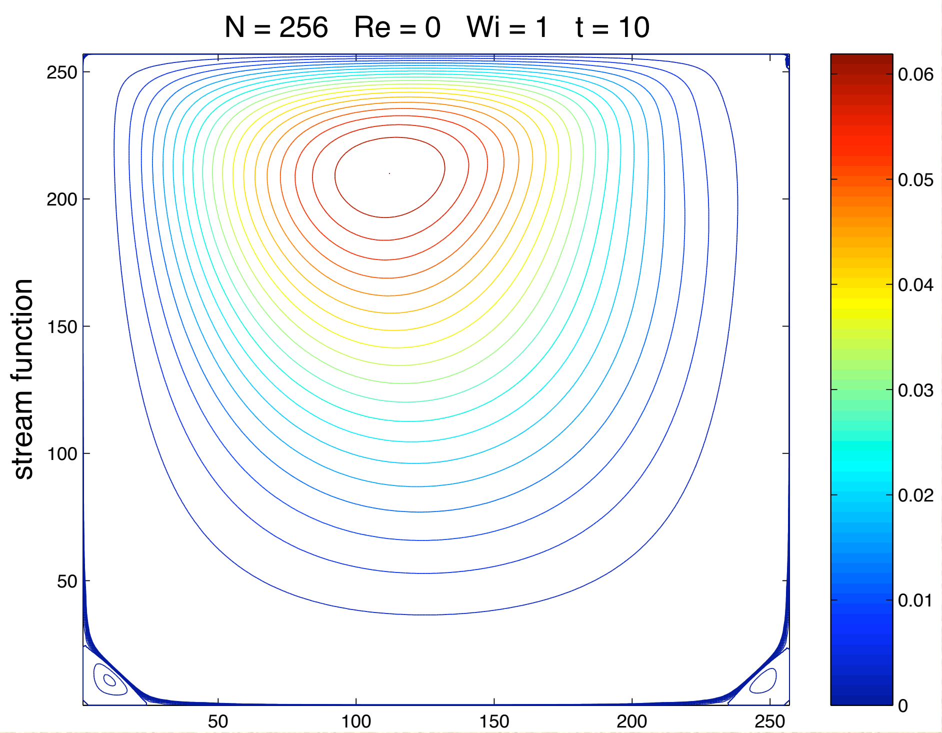
Lid-driven cavity

Lid-driven cavity

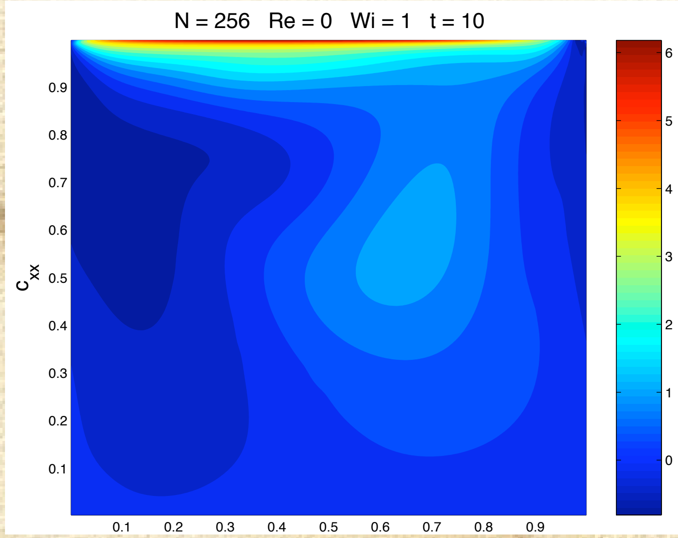


We=1

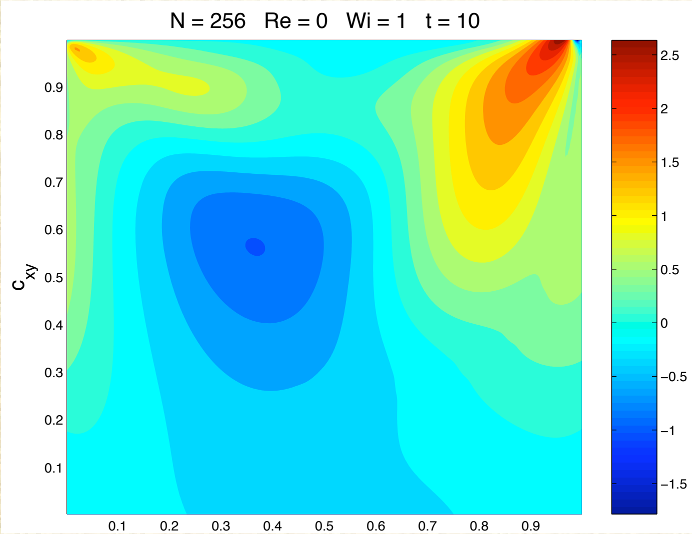
Solution converges to a steady state (would be symmetric for Stokes flow)



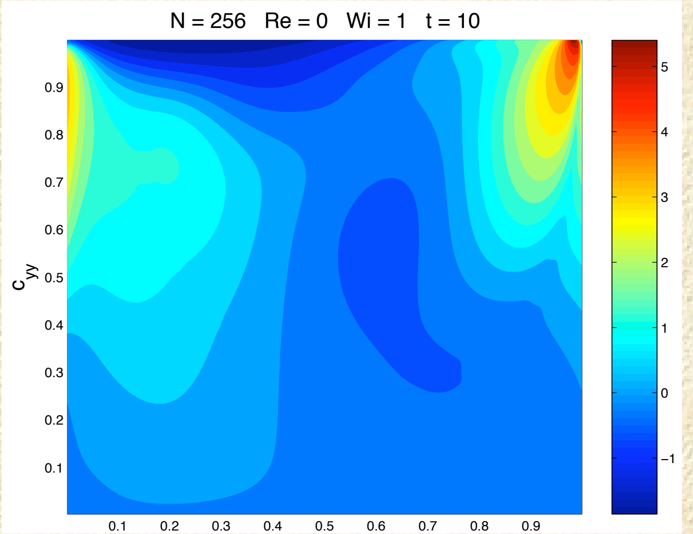
Stream function



ψ_{xx}



ψ_{xy}

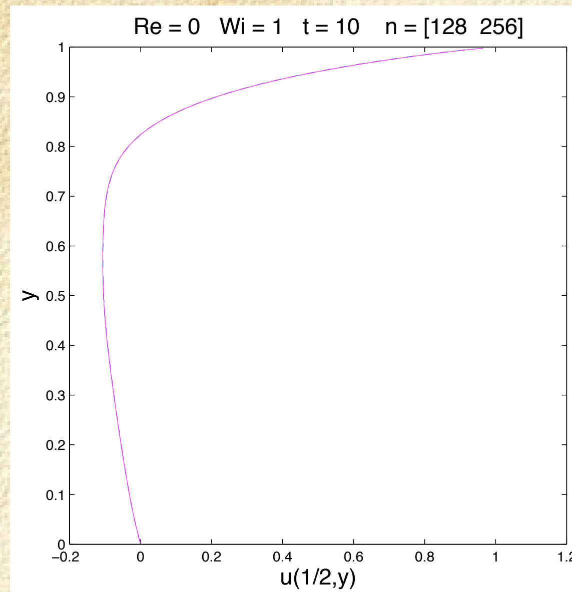


ψ_{yy}

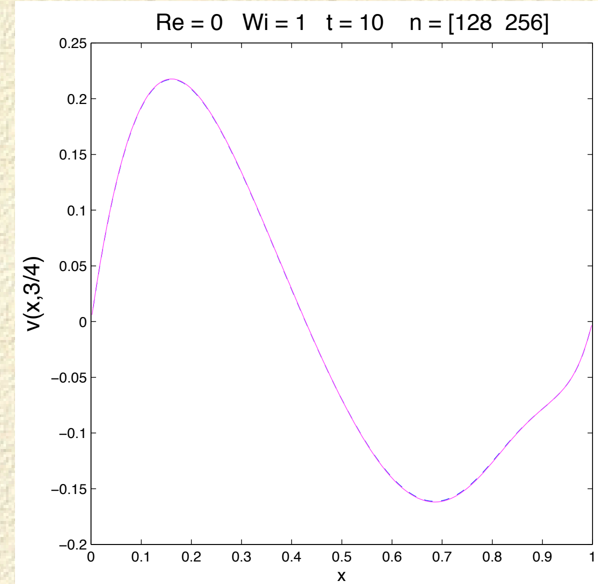
Numerical convergence analysis

	u			ψ_{xx}		
time	relative error N=64	relative error N=128	rate	relative error N=64	relative error N=128	rate
t=1	1.9×10^{-3}	3.7×10^{-4}	2.36	5.1×10^{-3}	1.1×10^{-3}	2.20
t=2	9.5×10^{-3}	2.1×10^{-3}	2.16	2.1×10^{-2}	5.1×10^{-3}	2.08
t=4	1.4×10^{-2}	5.1×10^{-3}	1.44	6.1×10^{-2}	1.8×10^{-2}	1.75

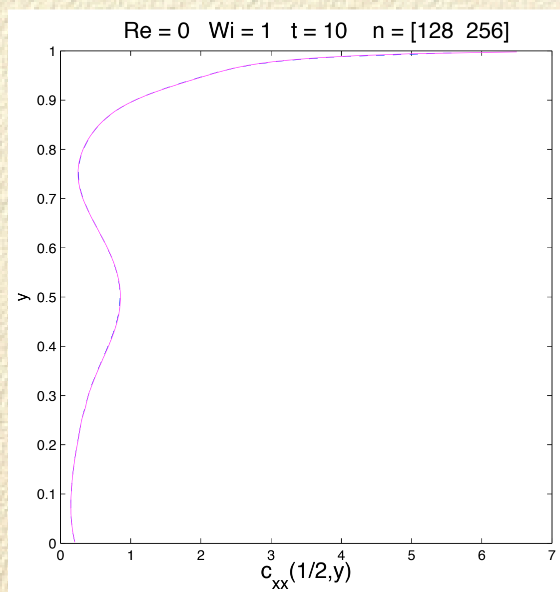
Comparison of data between 128x128 and 256x256 results



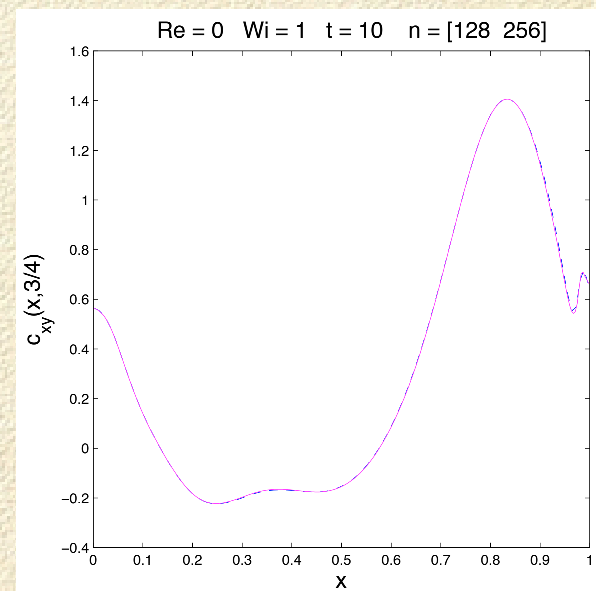
u(y) at x=1/2



v(x) at y=3/4



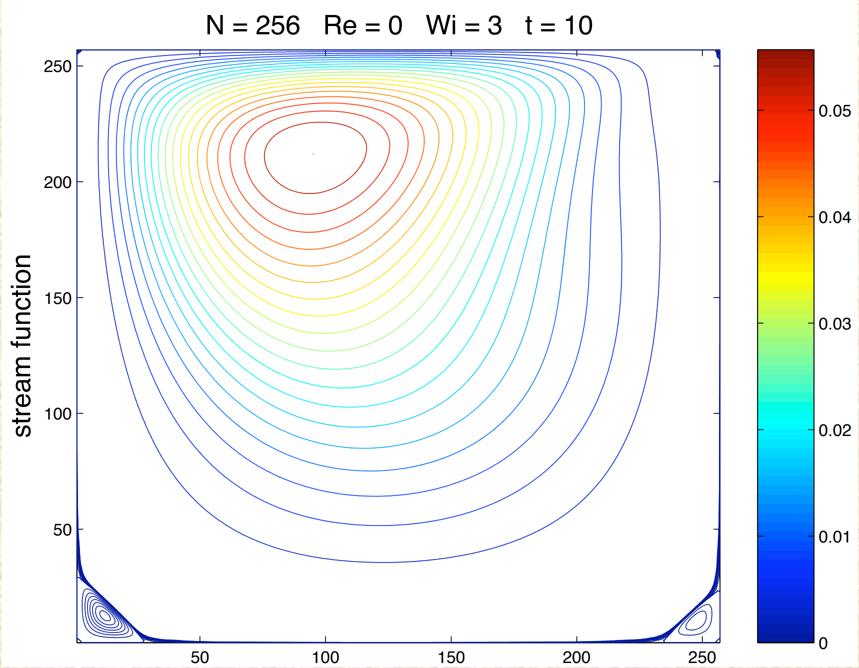
$\psi_{xx}(y)$ at x=1/2

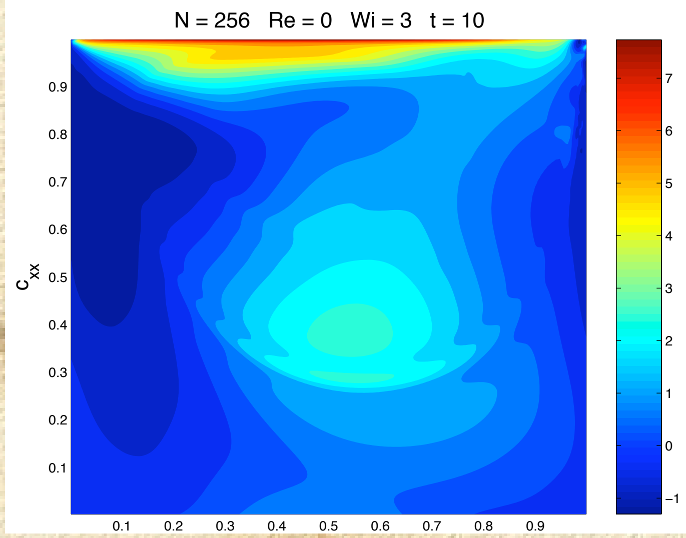


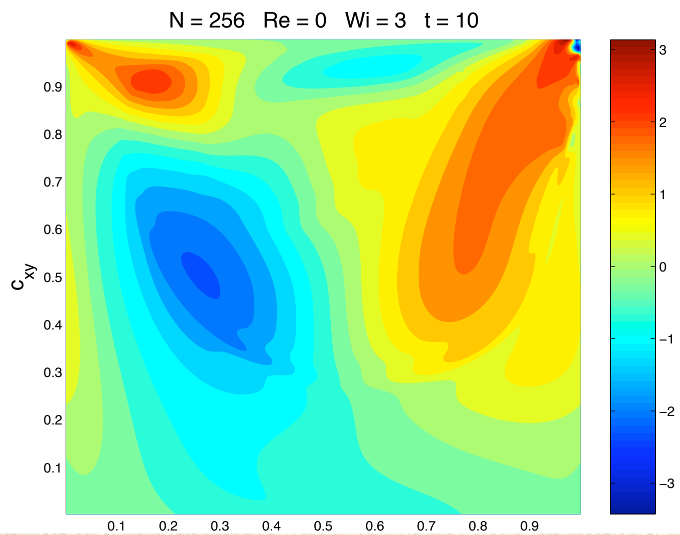
$\psi_{xy}(x)$ at y=3/4

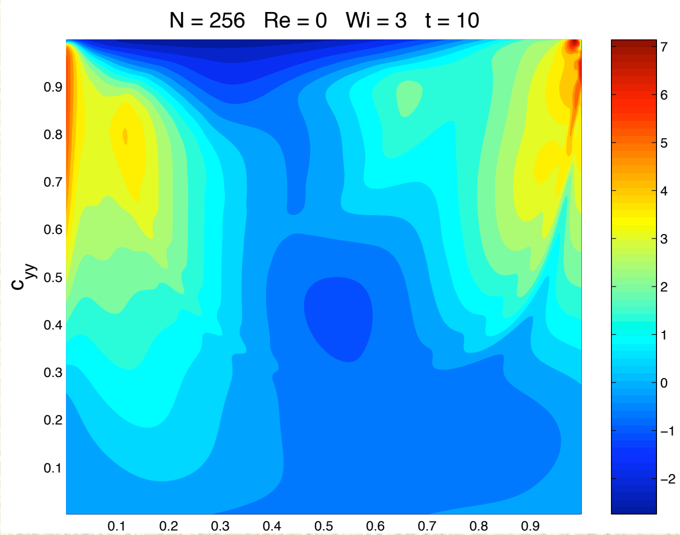
Results for higher *We*

We=3

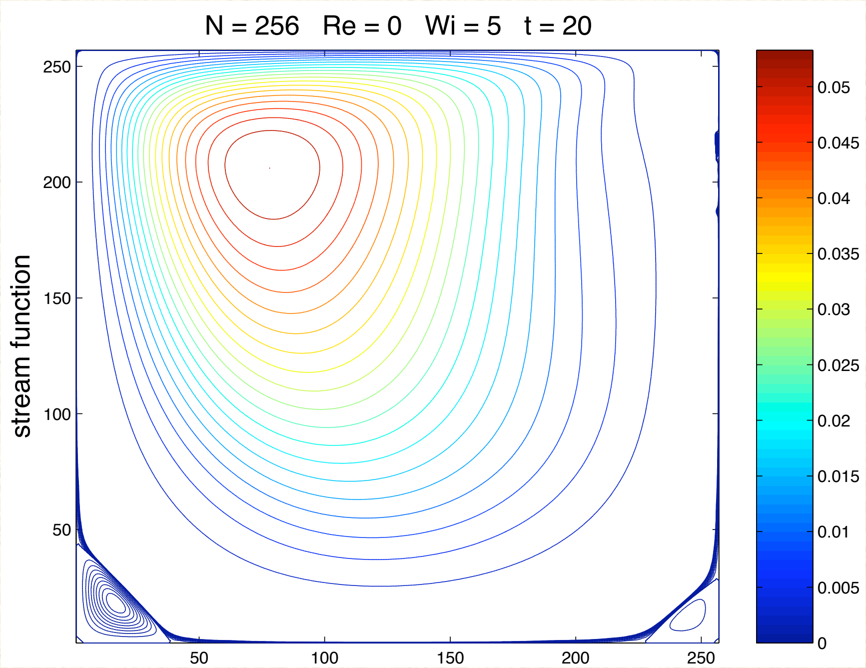


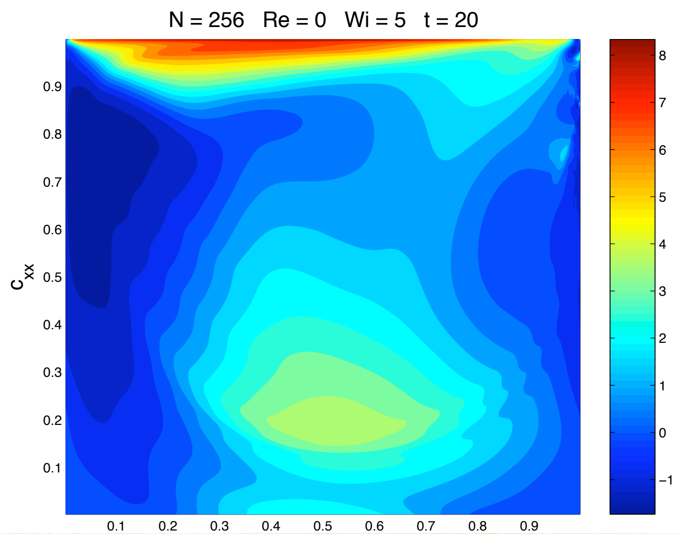


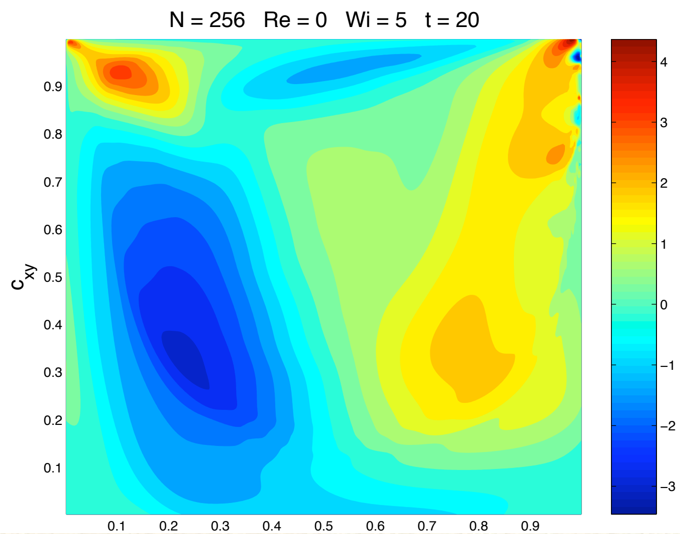


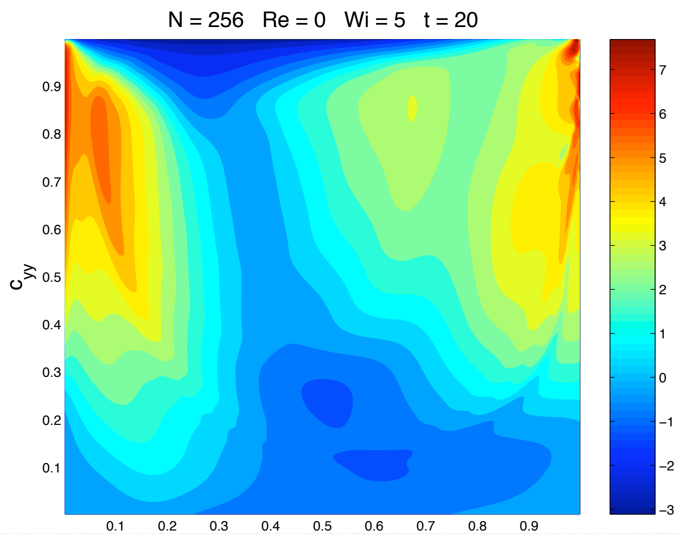


We=5


N = 256 Re = 0 Wi = 5 t = 20
stream function
250
200
150
100
50
50 100 150 200 250
0.05
0.045
0.04
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0


N = 256 Re = 0 Wi = 5 t = 20
c_{xx}
0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1
0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9
8 7 6 5 4 3 2 1 0 −1


N = 256 Re = 0 Wi = 5 t = 20
c_{xy}
0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1
0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9
4 3 2 1 0 −1 −2 −3


N = 256 Re = 0 Wi = 5 t = 20
c_{yy}
0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1
0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9
7 6 5 4 3 2 1 0 −1 −2 −3

Some remarks

1. Our results indicate that the HWNP *instability* is history
2. Works equally well with finite elements (Collaboration with Martien Hulsen)
3. Easily extended to particle tracking methods (e.g., Brownian configuration fields)
4. Method readily extended to nonlinear constitutive laws, and 3-dimensions
5. At high *We* loss of resolution and accuracy (back to standard numerical analysis...)
6. New horizons (*e.g., turbulent drag reduction*)

Epilogue

Time for the next speaker to prepare his/her transparencies

Find an acronym!!

High standards have been set by H.-C. Öttinger who invented CONFFESSITT (**C**alculation **O**f **N**on-**N**ewtonian **F**low: **F**inite **E**lements & **S**tochastic **SI**mulation **T**echniques)

What about MAL-COTE (**MA**trix **L**ogarithm of the **CO**nformation **TE**nsor)?