AERC 2006
3rd Annual European Rheology Conference
April 27-29, Hersonisos - Crete

PROGRESS IN COMPUTATIONAL RHEOLOGY WITH THE FINITE VOLUME METHOD

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OUTLINE:

- **Distinctive aspects of Computational Rheology**
- **Our activity in the field (1996-2005)**
- **Constitutive equations (differential)**
- **FVM (discretization)**
  - **Approximation of convective fluxes**
  - **Stress/velocity coupling**
- **Examples of results:**
  - ***Contraction* (*PTT* and *Old-B*) – *steady***
  - ***Cylinder* (*Old-B & FENE*) – *steady/unsteady instability***
  - ***Driven cavity* (*recoil: FENE*) – *unsteady***
  - ***Expansion* (*FENE-CR*) – *steady***
  - ***Vortex shedding* (*FENE*) – *unsteady***

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Many others have made progresses in Computational Rheology with FVM:

- Tanner, Phan-Thien, Xue, and co-workers
- Webster and co-workers (mixed FEM and FVM)
- Owens, Sahin (FVM pressure–free)

But the talk concentrates on review of our work...

RELEVANCE OF COMPUTATIONAL RHEOLOGY:

PRACTICAL APPLICATIONS

- Industry of thermoplastics (PVC, etc)
- Extrusion and Molding processes
- Paints (non-dripping)
- Glues (super-glues…)
- Food stuffs (yogurths; spaghetti; …)
- Cosmetics
- Two-phase flows
- Bioengineering: blood flow (hemodynamics)

DISTINGUISHING FEATURES OF COMPUTATIONAL RHEOLOGY :

- Elasticity and memory introduces a fluid time scale
- Level of elasticity measured by a Deborah number: $De = \lambda U / L$
- Additional equations for stresses (differential or integral)
- Stress equations are hyperbolic (full set, mixed type)
- Coupling between flow and constitutive eqs.
- Strength of coupling increases with "elasticity": $\beta = \eta_s / \eta_0$
- Stiff coupling in time dependent flows (2 time scales)
- Real fluids require complicate constitutive eqs.
- Multimode (6 eqs x N modes, giving 30 eqs. for 5 modes)

SCOPE OF OUR WORK:

- Extend tools of classical CFD to Computational Rheology
- Finite Volume Method
- Original code developed at Imperial College (*Oliveira, 1992*) (3D; non-orthogonal; non-staggered)
- Application to fundamental flows

ACHIEVEMENTS:

- General stress/strain solution code (many differential constitutive models)
- Method for stress/velocity coupling (stress at CV face)
- High Resolution Scheme (HRS) for stress equations
- Accurate results for some benchmark problems (contractions; expansions; cylinder; lid-driven cavity; etc)
- Ideas to improve the solution procedure (flow/stress linkage)

EQUATIONS:

- **Mass:** $$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \boldsymbol{u} = 0$$
- **Motion:**

$$\rho \frac{D\boldsymbol{u}}{Dt} = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \nabla \cdot \left[\eta_s (\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T) \right]$$

- **Constitutive (for the stress tensor τ):**

$$(\lambda \overset{\triangledown}{\boldsymbol{\tau}}) \quad \lambda \overset{\triangledown}{\boldsymbol{\tau}} + \boldsymbol{\tau} = 2\eta \mathbf{D}$$

- **Oldroyd derivative:** $\overset{\triangledown}{\boldsymbol{\tau}} = \frac{D\boldsymbol{\tau}}{Dt} - (\boldsymbol{\tau} \cdot \nabla \boldsymbol{u} + \nabla \boldsymbol{u}^{\mathrm{T}} \cdot \boldsymbol{\tau})$

EXAMPLES OF CONSTITUTIVE MODELS (1):

- **Newtonian:** $\boldsymbol{\tau} = 2\mu\mathbf{D} = \mu\left(\nabla\mathbf{u} + \nabla\mathbf{u}^{\mathrm{T}}\right)$

- **Generalized Newtonian Fluid (GNF):** $\boldsymbol{\tau} = \eta(\dot{\gamma})\left(\nabla\mathbf{u} + \nabla\mathbf{u}^{\mathrm{T}}\right)$

  viscosity model: $\eta(\dot{\gamma}) = K\,\dot{\gamma}^{\,n-1}$

- **Differential Viscoelastic:**

$$\boldsymbol{\tau} + \lambda_{eq}\left(\frac{\partial\boldsymbol{\tau}}{\partial t} + \nabla\cdot(\mathbf{u}\boldsymbol{\tau})\right) = \eta_{p,eq}\left(\nabla\mathbf{u} + \nabla\mathbf{u}^{T}\right) + \lambda_{eq}\left(\boldsymbol{\tau}\cdot\nabla\mathbf{u} + \nabla\mathbf{u}^{T}\cdot\boldsymbol{\tau}\right)$$

$$\lambda_{eq} \equiv \lambda / f(\tau) \qquad \eta_{p,eq} \equiv \eta_p / f(\tau)$$

EXAMPLES OF CONSTITUTIVE MODELS (2):

- **Oldroyd-B:** $f(\tau) = 1 \Leftrightarrow \begin{cases} \lambda_{eq} \equiv \lambda \\ \eta_{p,eq} \equiv \eta_p \end{cases}$

- **UCM: Upper Convected Maxwell** $\eta_s = 0$

- **FENE-CR:** $\begin{cases} \lambda_{eq} \equiv \lambda / f(\tau) \\ \eta_{p,eq} \equiv \eta_p \end{cases}$

$$f(\tau) = \frac{L^2 + \dfrac{\lambda}{\eta_p} tr(\boldsymbol{\tau})}{L^2 - 3}$$

- **PTT Linear:** $f(\tau) = 1 + \varepsilon\dfrac{\lambda}{\eta_p} tr(\boldsymbol{\tau})$

shear-thinning

- **PTT Exponential:** $f(\tau) = \exp\left[\varepsilon\dfrac{\lambda}{\eta_p} tr(\boldsymbol{\tau})\right]$

EXAMPLES OF CONSTITUTIVE MODELS (3):

- **FENE-P:** $f(\tau) = 1 + \frac{3}{b+2}\left[1 + \frac{\lambda}{3a\eta_p} tr(\boldsymbol{\tau})\right]$

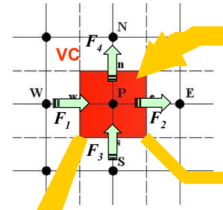
$$\begin{cases} \lambda_{eq} \equiv \lambda / f(\tau) \\ \eta_{p,eq} \equiv \eta_p / (f/a); a \equiv (b+5)/(b+2) \end{cases}$$

additional term: $\ldots = \ldots - \frac{D(1/f)}{Dt}\left(\lambda\boldsymbol{\tau} + a\eta_p \mathbf{I}\right)$

- **Giesekus:** $\begin{cases} \boldsymbol{\tau} + \lambda\left(\overset{\nabla}{\boldsymbol{\tau}} + \frac{\alpha}{\eta_p}\boldsymbol{\tau}\cdot\boldsymbol{\tau}\right) = 2\eta_p \mathbf{D} \\ f(\tau) = 1 \end{cases}$

shear-thinning

FINITE VOLUME METHOD (1):



$$\lambda\tau_{ij} + \left(\frac{\partial \tau_{ij}}{\partial t} + u_k \frac{\partial \tau_{ij}}{\partial x_k}\right) = \eta\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \left(\tau_{ik}\frac{\partial u_j}{\partial x_k} + \tau_{jk}\frac{\partial u_i}{\partial x_k}\right)$$

Mass conservation: (mass fluxes)

$$\sum_{f=1}^{6} F_f = 0 \qquad F_f = \sum_{f=1}^{3} \rho B_{fj} \tilde{u}_j^{(n+1)}$$

Momentum conservation:

2º $a_P \boldsymbol{u}_P^{**} = \sum_{F=1}^{6} a_F \boldsymbol{u}_F^{**} + \left\{-\nabla p^* + S_u[\nabla\cdot\tilde{\boldsymbol{\tau}}^{(n+1)}] + S_u^{HOS} + \frac{\rho V}{\Delta t}\left(2.0\boldsymbol{u}_P^{(n)} - 0.5\boldsymbol{u}_P^{(n-1)}\right)\right\}$

Stress evolution: **source terms**

1º $a_P^\tau \boldsymbol{\tau}_P^{(n+1)} = \sum_{F=1}^{6} a_F^\tau \boldsymbol{\tau}_F^{(n+1)} + \left\{S_\tau[\nabla \boldsymbol{u}^*] + S_\tau^{HOS} + \frac{\lambda_{ef} V}{\Delta t}\left(2.0\boldsymbol{\tau}_P^{(n)} - 0.5\boldsymbol{\tau}_P^{(n-1)}\right)\right\}$

Time advancement: 2nd order backward scheme

(*Oliveira, Pinho, Pinto 1998; Oliveira 2001*)

FINITE VOLUME METHOD (2):

- Large sets of linearised equations *A.x=b* solved with pre-conditioned conjugate gradient solvers.

- Pressure–correction method (SIMPLEC).
  $\left(p' = p^{**} - p^{*}\right)$ (akin to projection methods)

$$\boldsymbol{u}_P^{(n+1)} = \boldsymbol{u}_P^{**} - \frac{1}{a_P}\nabla p'$$

$$\nabla \bullet \left(\frac{1}{a_P}\nabla p'\right) - \left\{\nabla \bullet \boldsymbol{u}_P^{**}\right\} = 0$$

- Non-linearities dealt with by iteration.
  (inside a time step, for time dependent calculations)

FINITE VOLUME METHOD (3):

Numerical Issues:

- A – Stress/velocity coupling.

- B – Discretization of convective fluxes.

A - STRESS/VELOCITY COUPLING METHOD:

- **Term needed in *u*-eq.:** $\nabla \cdot \boldsymbol{\tau} \rightarrow \sum_{f=1}^{6} \sum_{j=1}^{3} B_{fj} (\tilde{\tau}_{ij})_f = \sum_{f=1}^{6} T_{fi}$

- **Write stress eq.:as:**

$$a_P^{\tau} \tau_{ijP} = \sum a_F^{\tau} \tau_{ijF} + \sum_{l=1}^{3} \left(b_{li} \left[\Delta u_j \right]_l + b_{lj} \left[\Delta u_i \right]_l \right) + S_{ij}^{\tau}$$

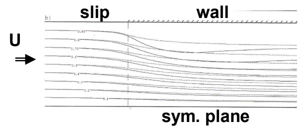
$$a_P^{\tau} \boldsymbol{\tau}_P^{(n+1)} = \sum_F a_F^{\tau} \boldsymbol{\tau}_F^{(n+1)} + S_{\tau}[\nabla \boldsymbol{u}] + S_{\tau}^{HOS} + \frac{\Delta V}{\Delta t} \left\{ 2.0 \boldsymbol{\tau}_P^{(n)} - 0.5 \boldsymbol{\tau}_P^{(n-1)} \right\}$$

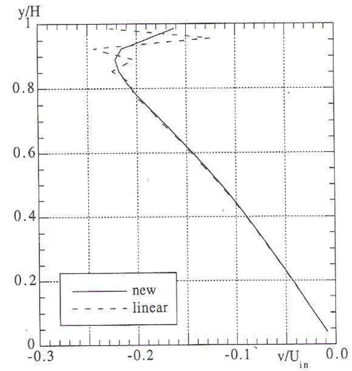
where: $b_{li} = \eta B_{li} + \lambda \sum_{k=1}^{3} B_{lk} \tau_{ik}$ and B_{li} are areas

- **Divide by central coeff.** a_P^{τ} **and interpolate:**

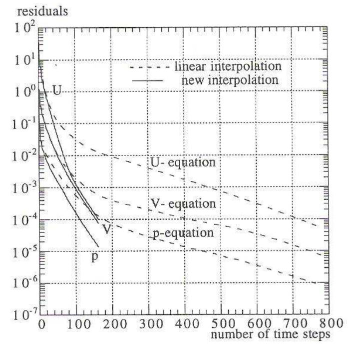
$$\tilde{\tau}_{ij} = \overline{\sum a'_F \tau_{ijF}} + \overline{\sum_{l \neq f}^{2} \left(b'_{li} \left[\Delta u_j \right]_l + b'_{lj} \left[\Delta u_i \right]_l \right)} + \tilde{b}'_{fi} \left[\Delta u_j \right]_f + \tilde{b}'_{fj} \left[\Delta u_i \right]_f + \overline{S}'^{\tau}_{ij}$$

EXAMPLE:





Vertical profile of v-velocity in entry flow



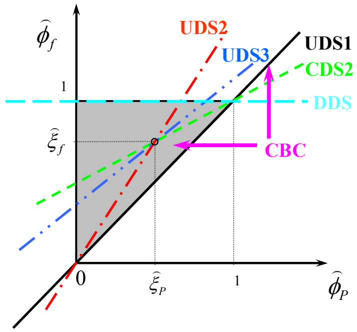
Residuals of equations

Slip/Stick Flow

B - CUBISTA: HIGH RESOLUTION SCHEME (1):

Calculation of cell-face flux:

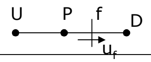
$$\boxed{F_f \phi_f}$$



- Important for accuracy
- Upwind (UDS1) too inaccurate
- High Order (HOS): oscillations
- Avoid oscillations: HRS
- Problem: iterative convergence

(B.P. Leonard)

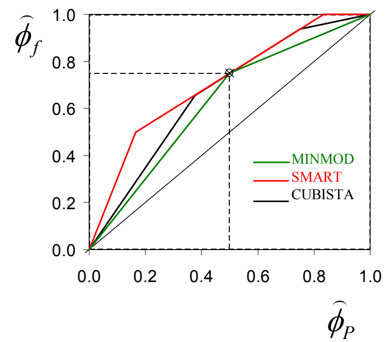
HOS in Normalised Variable Diagram (NVD): $\hat{\phi} = \dfrac{\phi - \phi_U}{\phi_D - \phi_U}$



B - CUBISTA: HIGH RESOLUTION SCHEME (2):

Definition of scheme:

$$\hat{\phi}_f = \begin{cases} \frac{7}{4}\hat{\phi}_P & 0 < \hat{\phi}_P < \frac{3}{8} \\ \frac{3}{4}\hat{\phi}_P + \frac{3}{8} & \frac{3}{8} \le \hat{\phi}_P \le \frac{3}{4} \\ \frac{1}{4}\hat{\phi}_P + \frac{3}{4} & \frac{3}{4} < \hat{\phi}_P < 1 \\ \hat{\phi}_P & \text{elsewhere} \end{cases}$$



(based on TVD restrictions)

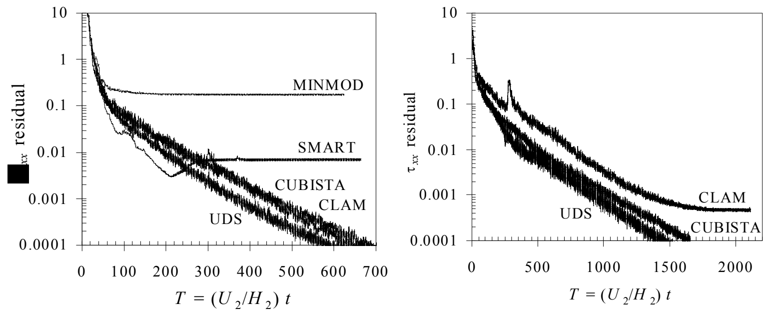
$\hat{\phi}_f \le (2-C)\hat{\phi}_P ; C = 0$

we chose: $C = 0.25$

(*Alves, Oliveira, Pinho, IJNMF 2003*)

B - CUBISTA: HIGH RESOLUTION SCHEME (3):

Contraction flow, UCM, De=3



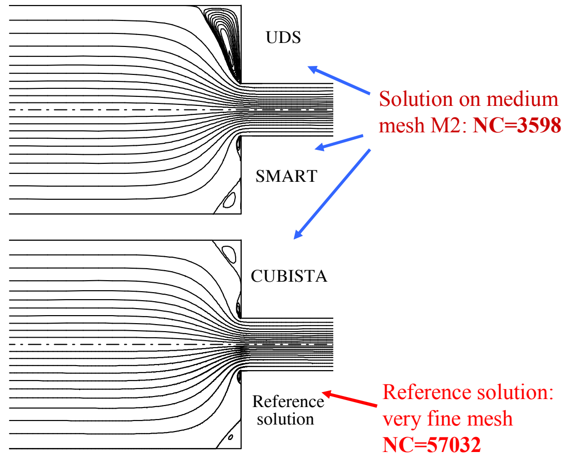
Mesh M2

(NC=3598, Dx=0.02)

Mesh M3

(NC=14258, Dx=0.01)

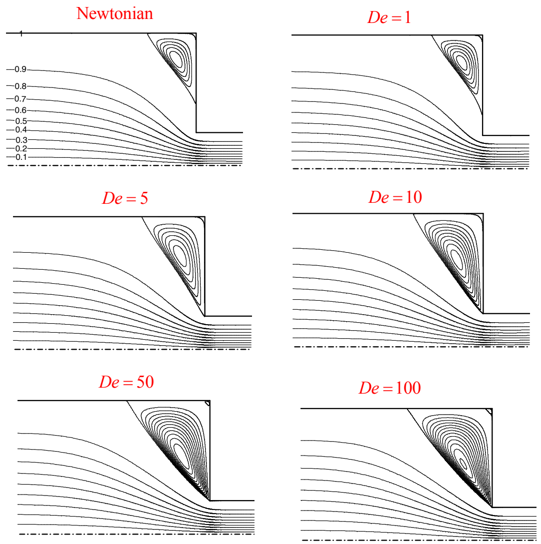
B - CUBISTA: HIGH RESOLUTION SCHEME (4):



EXAMPLES OF CALCULATIONS:

- Flow through contractions
- Flow around confined cylinder
- Lid-Driven cavity flows
- Flow through expansions
- Vortex shedding behind unbound cylinder
- Pulsating pressure gradient

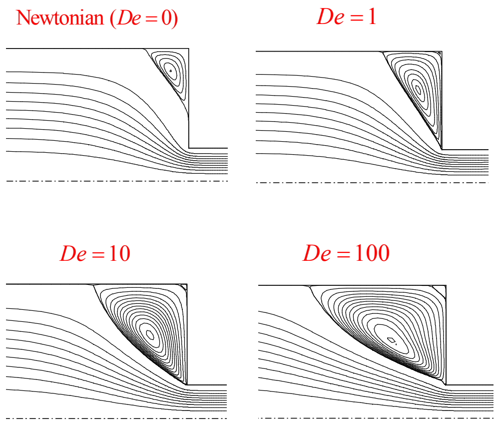
4:1 PLANAR CONTRACTION FLOW, PTT LINEAR



model parameters:
$\varepsilon = 0.25; \quad \beta = 1/9$

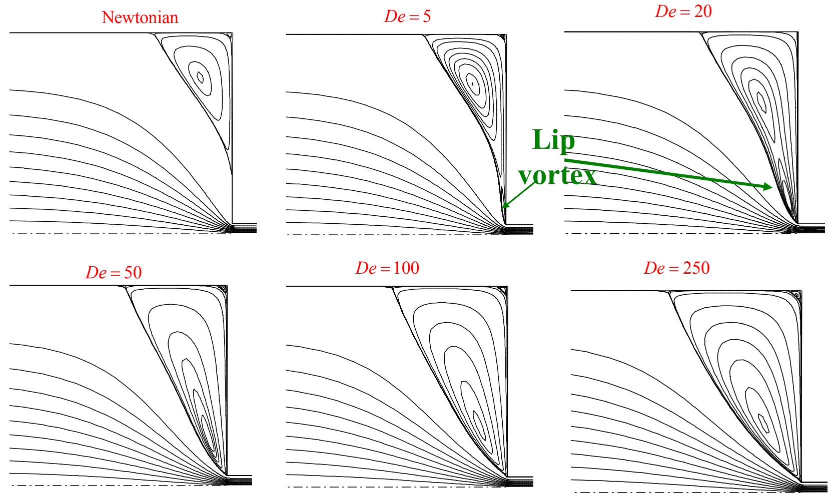
(*Alves, Oliveira, Pinho, JNNFM 2003*)

4:1 AXISYMMETRIC CONTRACTION FLOW, PTT LINEAR



(*Alves, Pinho, Oliveira, ENCIT 2004*)

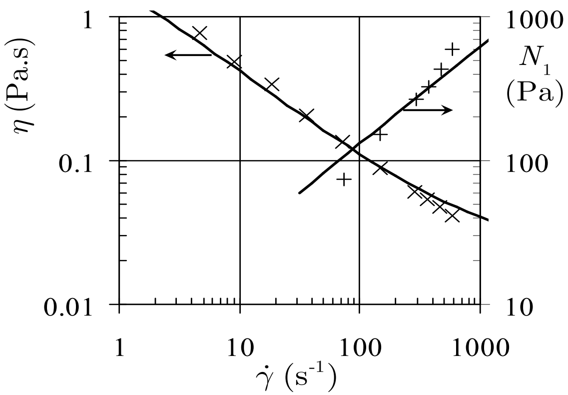
20:1 PLANAR CONTRACTION FLOW, PTT LINEAR



(*Alves, Oliveira, Pinho, JNNFM 2004*)

Comparison with experiments, 16:1
(*Evans & Walters 1986*)

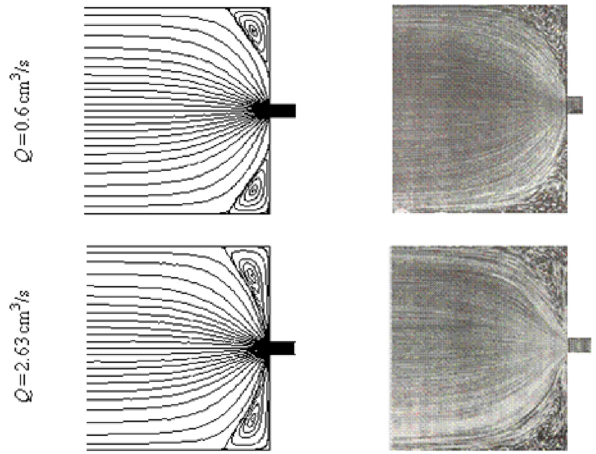
1% polyacrylamide in water fitted with a PTT

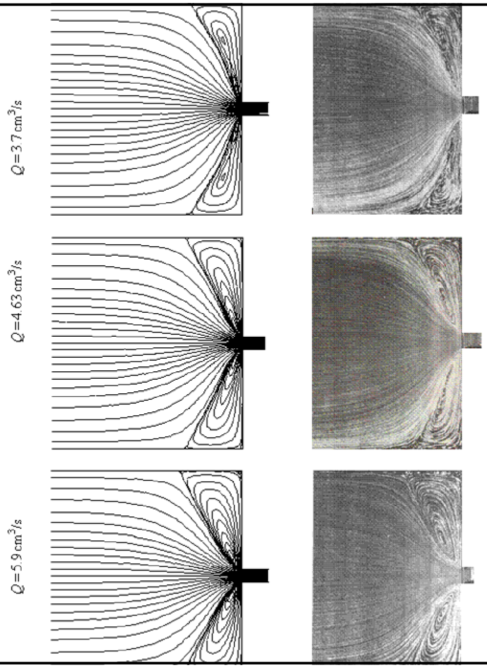


$\varepsilon = 0.25$; $\beta = 1/120$

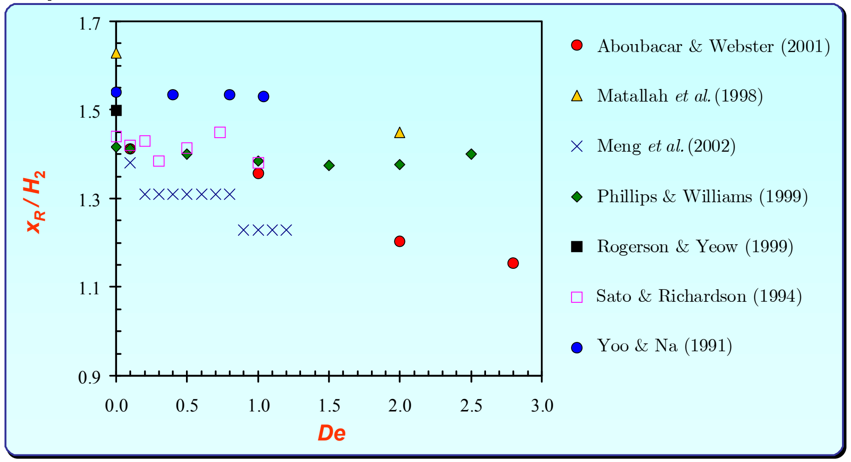
$\lambda = 2.0$ s; $\eta_0 = 2.5$Pa.s

Comparison with experiments, 16:1
(*Evans & Walters 1986*)



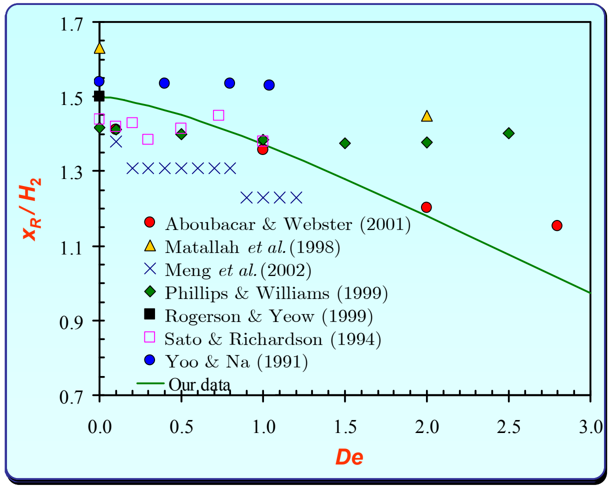


4:1 CONTRACTION FLOW, OLDROYD-B:



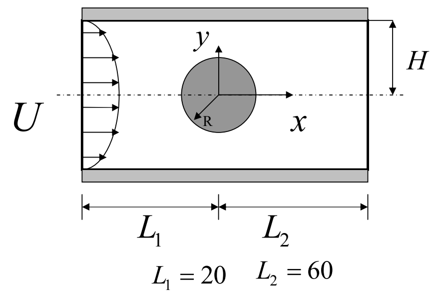
(benchmark since 1988)

4:1 CONTRACTION FLOW, OLDROYD-B:



Alves, Oliveira, Pinho, JNNFM (2000; 2003)

THE CONFINED CYLINDER BENCHMARK:



"blockage":

$B = R / H = 0.5$

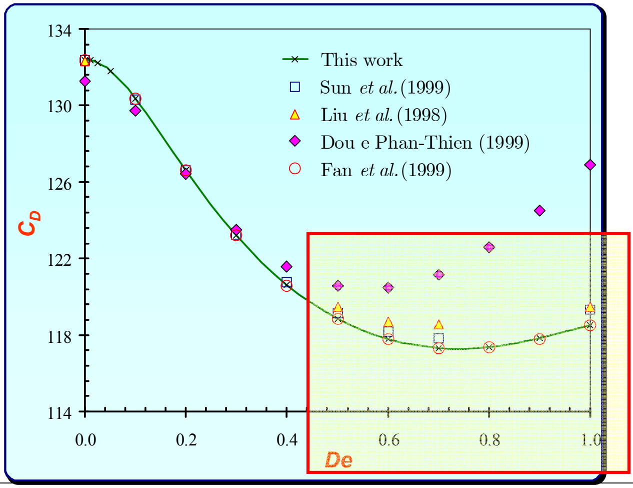
$De = \lambda U / R$

$Re = 0$

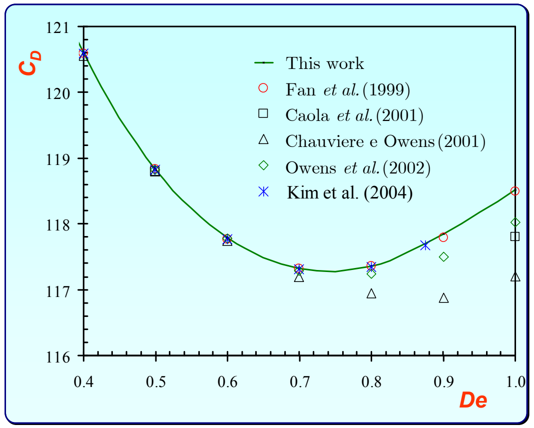
(benchmark since 1994)

CONFINED CYLINDER WITH OLDROYD-B:

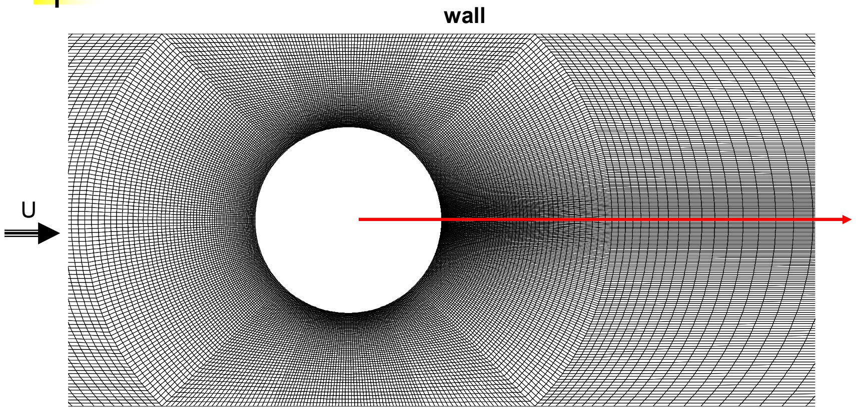
Initial calculations: *Alves, Pinho, Oliveira, JNNFM* (*2001*)



CONFINED CYLINDER WITH OLDROYD-B:



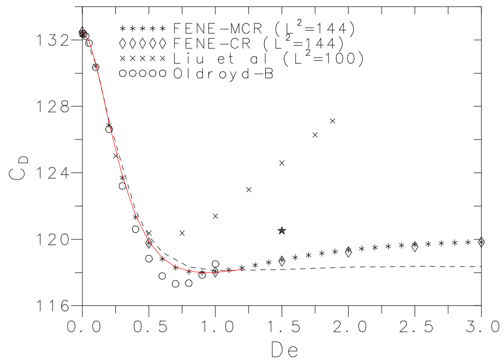
FENE-CR CALCULATIONS: example of mesh



Zoom in -3<x<5; **M60(WR)-FO**

- refined along wake
- full domain
- row of cells along wake

STEADY FLOW: DRAG COEFFICIENT (FENE-CR)



L^2
extensibility parameter

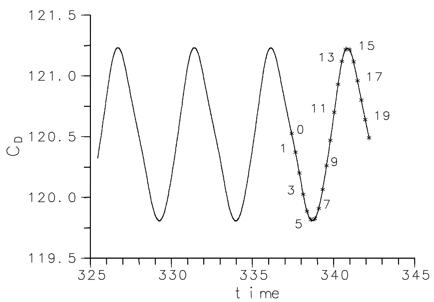
Red: L^2=144
Dash: L^2=100
(finer mesh)

Sahin, Owens

(Oliveira & Miranda, JNNFM 2005)

UNSTEADY REGIME – DRAG vs. TIME:

Natural Instability (Hopf)

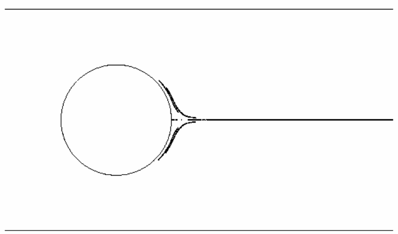


$\Delta t = 2.4 \times 10^{-3}$

$T \approx 4.7$

De=1.5; Re=0; L^2=144; β =0.59

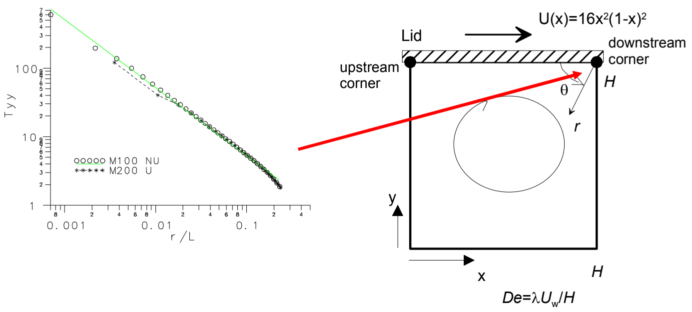
EXAMPLE OF STREAKLINES, DE=1.5:



Note: no ondulation

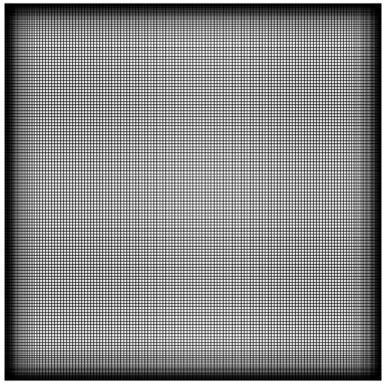
LID-DRIVEN CAVITY:

Unregularized (Newt.), U=const



(Oliveira, IWNMNNFM 2005)

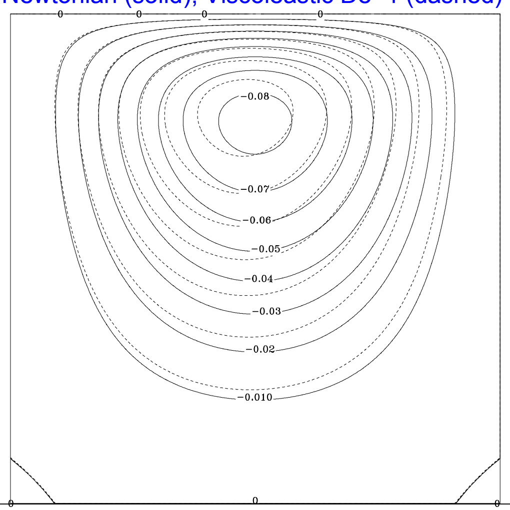
MESH-4: 160x160 NU



$$\Delta x_{\min} = 1.0 \times 10^{-3}$$

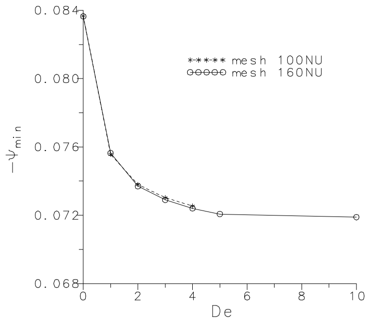
STREAMLINE COMPARISON:

Newtonian (solid), Viscoleastic De=1 (dashed)

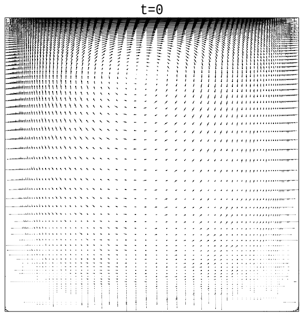


Pakdel et al.
PoF 1998

VARIATION OF MAIN EDDY RECIRCULATION WITH ELASTICITY:



TIME DEPENDENT FLOW: RECOIL FROM De=2



N1-steady

Velocity Vectors

Streamlines

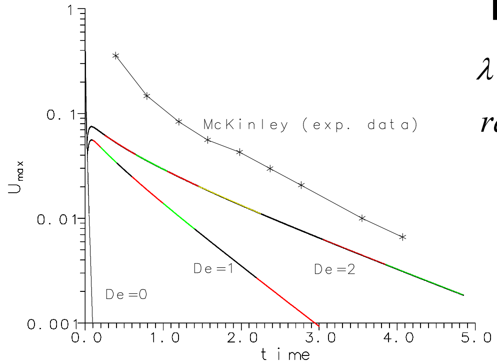
De=2; Mesh 4

$\Delta t = 0.5 \times 10^{-4}$

up to:

$\Delta t = 5 \times 10^{-4}$

DECAY OF MAXIMUM VELOCITY IN CAVITY:



McKinley:

$\lambda = 1.6s; rate = 1.13s$

$rate / \lambda = 0.71$

De=0, T=0.019

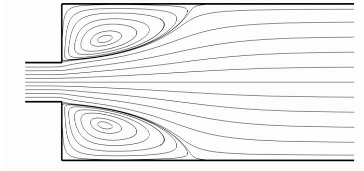
De=1, T=0.75

De=2, T=1.48

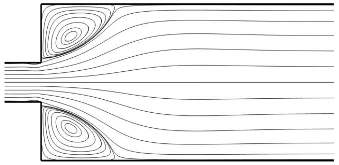
T/De=0.75; 0.74

FLOW THROUGH EXPANSIONS (1:4):

De=0

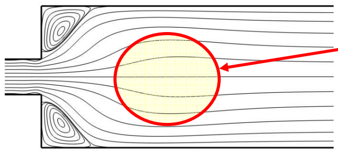


De=2



FENE-CR, L^2=100, β=0.5, Re=20

De=5



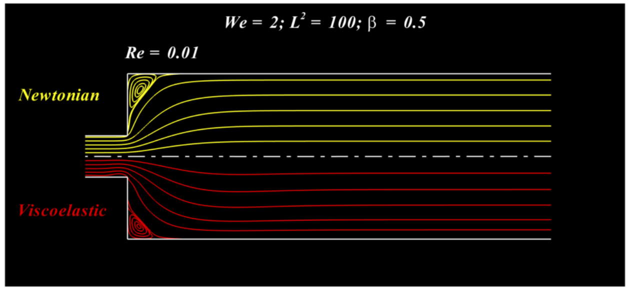
Bulging of streamlines

E=De/Re

(*Rocha & Oliveira, 2005*)

1:4 PLANAR EXPANSION:

Re ≤ 35, no bifurcation



EFFECT OF POLYMER CONCENTRATION (β):

C=(1/ β)-1

Newtonian case:
Re = 20; *We* = 0; L^2 = 100

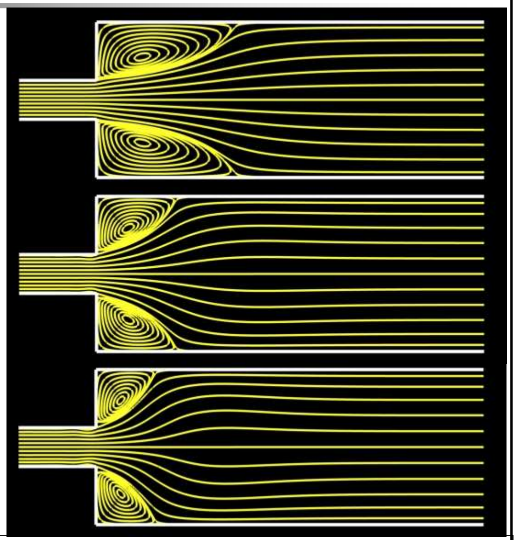
$\beta = 1.0$

Viscoelastic case 1:
Re = 20; *We* = 2; L^2 = 100

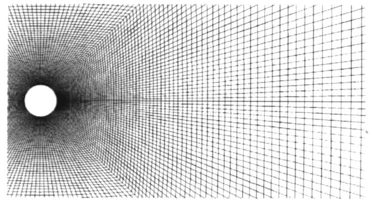
$\beta = 0.5$

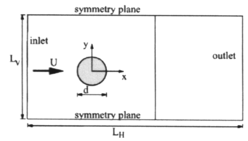
Viscoelastic case 2:
Re = 20; *We* = 2; L^2 = 100

$\beta = 0.3$



VORTEX SHEDDING BEHIND UNCONFINED CYLINDER: mesh & flow domain





$$Re = \frac{\rho U d}{\eta_0} = 100$$

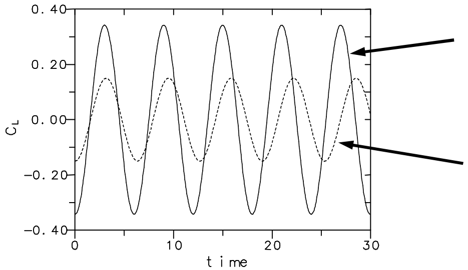
$$De = \frac{\lambda U}{d} = 0 - 80$$

$$L^2 = 100$$

$$c = 0.1; \beta = 0.909$$

FENE-CR : constant-viscosity elastic liquid

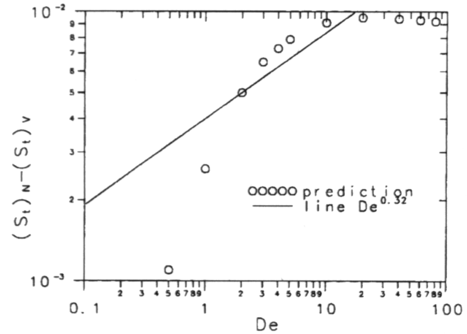
VORTEX SHEDDING BEHIND UNCONFINED CYLINDER: effect on lift



Lift coefficient versus time
De=80, L^2=100, Re=100

- period: +5.8%
- magn. lift: -56 %
- magn. drag: -83%

VORTEX SHEDDING BEHIND UNCONFINED CYLINDER: effect on frequency



Decay of Strouhal number

Data: Usui et al 1980.

St=f.d/U

De up, freq. down

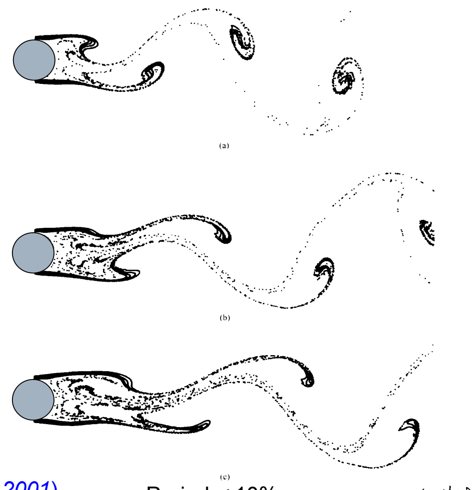
VORTEX SHEDDING BEHIND UNCONFINED CYLINDER: effect of elasticity (De)

Newt.

$\Delta t = 0.025$

FENE-CR
L^2=1200
Re=100
c=0.1

$\Delta t = 0.0125$



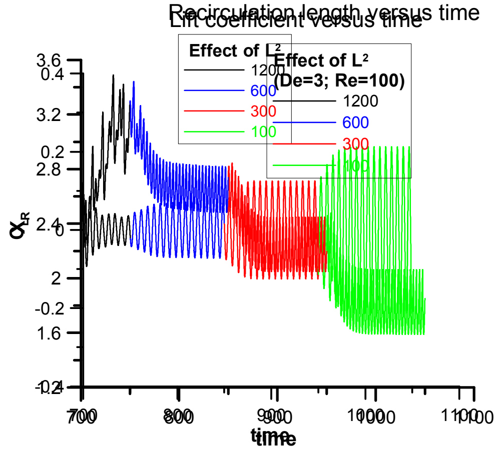
(Oliveira,JNNFM 2001)

Period: +10%

VORTEX SHEDDING BEHIND UNCONFINED CYLINDER: effect of L^2 on lift & vortices

FENE-CR
Effect of Extensibility

Constant:
Deborah, De=3
Reynolds, Re=100
Concentration, c=0.1



L^2=100, 300, 600, 1200
From top to bottom

VORTEX SHEDDING BEHIND UNCONFINED CYLINDER:

FENE-CR
Effect of Concentration

Constant:
- Deborah, De=3
- Reynolds, Re=100
- Extensibility, L^2=100

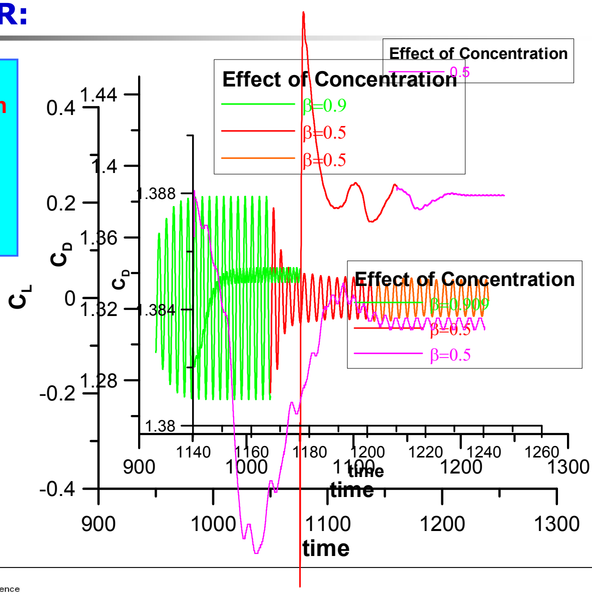
Drag versus time when concentration raises from c=0.1 to c=1

$$\beta = \frac{\eta_S}{\eta_0} = \frac{1}{1+c}$$

$$c = \frac{\eta_P}{\eta_S} = \frac{1}{\beta} - 1$$

c=0.1; 1.0; 2.3

c=4.0



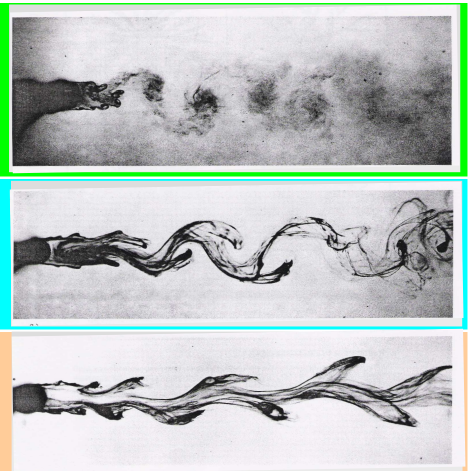
VORTEX SHEDDING BEHIND UNCONFINED CYLINDER:

Visualisations in Boger and Walters (by Strauss & Dohmann, TSF 1991): Re=5000

Water:

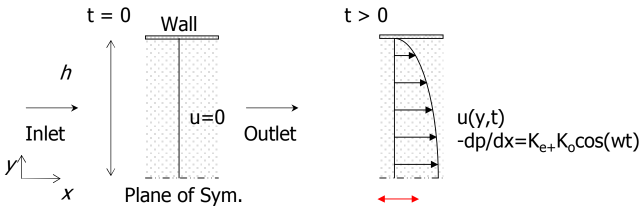
50 ppm PAC

1000 ppm surfactant



UCM FLOW IN CHANNEL DUE TO PULSATING PRESSURE-GRADIENT (1):

- **"Simple" 1D unsteady flow**
- **Analytical solution available**
- **Very convenient to assess and develop methods**
- **Relevance to blood flow**
- **More complicate than "startup flow"**



UCM FLOW IN CHANNEL DUE TO PULSATING PRESSURE-GRADIENT (2):

Elasticity number, E=1
Womersley number, α=4.9

$$\alpha = h\sqrt{\frac{\omega}{\eta_o/\rho}}$$

Comparison with theory

Simulation results for a period

Line: simulations

Symbols: theory

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FUTURE WORK:

- Near-wall treatment
- Devise a “log-law” for stresses
- Evaluation of gradients
- Use Log(stress)   (Fattal & Kupferman, 2005)
- 3D Calculations at high De
- Implement compressibility (unsteady and moving mesh) (sugges. Mackley) (Webster et al)

ACKNOWLEDGMENTS:

Prof. M.P. Escudier and Dr. R.J. Poole (Univ. Liverpool)

Engs. Gerardo N. Rocha (UBI) and Amílcar Miranda (UBI)

Ms. Ana Sofia Duarte (UBI)

FCT Fundação para a Ciência e a Tecnologia
MINISTÉRIO DA CIÊNCIA, INOVAÇÃO E DO ENSINO SUPERIOR Portugal

Project POCTI/EME/48665/2002