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Finite volume method for the prediction of viscoelastic flows with compressibility effects

P. J. Oliveira and A. S. R. Duarte

University of Beira Interior
Electromechanical Engineering Dep.
MTP R&D Unit

Abstract

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Implement compressibility into an existing finite volume method (FVM) procedure

- Explanation of the basis of the methodology (borrowed from CFD with FVM) and difficulties encountered (Boundary conditions, non-symmetric matrix, …).

- Application of the methodology to a simple test case: channel flow with prescribed inlet velocity (Newtonian and FENE-MCR* fluids).

* - *Finite extensible nonlinear elastic – modified Chilcott-Rallison.*

Motivation

Compressible flows play an important role, occuring widely in nature and in many industrial processes:

Injection blow moulding

High speed extrusion

- Incompressible assumption fails in cases of time-dependent flows at high pressures (the usual situation in extrusion processes).
- Compressibility effects in unsteady capillary flow: - pressure buildup and relaxation; -pressure variation during the occurence of “spurt” instabilities.

Previous works

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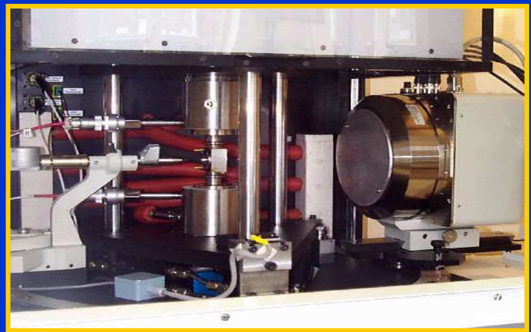
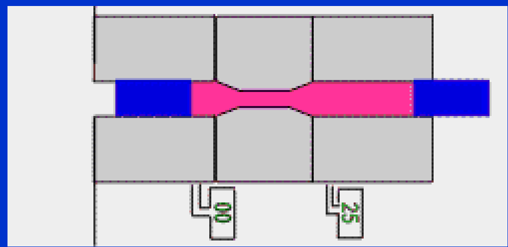
G. C. Georgiou and M. J. Crochet, J. Rheol.38(3) (1994) 639-654.

Study of time-dependent compressible flows of Newtonian fluids using arbitrary nonlinear slip law relating the shear stress to the velocity at the wall.

M. Ranganathan, M. R. Makley, P. H. Spitteler, J. Rheol.43(2) (1999) 443-451.

Experimental data on the time-dependent capillary flow measurements for a high-density polyethylene using the multipass rheometer (MPR)=> pressure and stress relaxation upon cessation of pistons are due to compressibility.





I. J. Keshtiban, F. Belblidia, M. F. Webster, J. N. Newt Fluid Mech. 122 (2004) 131-146.

Finite element method accomodating low Mach number compressile and incompressible viscoelastic fluids.

Focus on steady flows showing the influence of compressibility on temporal, monotonic, in-phase convergence properties.

Governing Equations

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- Conservation equations

Mass

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0$$

Momentum

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial}{\partial x}(\rho u u) =$$

$$= -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x}\left(\eta_s \frac{\partial u}{\partial x}\right) + \frac{\partial \tau}{\partial x}$$

- Constitutive model – FENE-MCR

$$\tau + \frac{\lambda}{f(\tau)}\overset{\nabla}{\tau} = 2\eta_p D$$

$$f(\tau) = \frac{L^2 + \left(\lambda/\eta_p\right) tr(\tau)}{L^2 - 3}$$

$$\boxed{\beta = \frac{\eta_s}{\eta_0} \qquad \eta_0 = \eta_s + \eta_p}$$

Compressibility

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Physical Definition: the speed of propagation of longitudinal acoustic waves transmitted through the flow takes on finite values.

$$K = \frac{1}{\rho}\left(\frac{\partial \rho}{\partial p}\right)_T$$

Isothermal compressibility coefficient

Upon integration, gives equation of state linking density and pressure:

$$K = \frac{1}{\rho_0}\left(\frac{\rho - \rho_0}{p - p_0}\right) \Leftrightarrow \rho = \rho_0\left[1 + K\left(p - p_0\right)\right]$$

p_0 and ρ_0: reference values

$K \approx 1.5\text{x}10^{-9}$ [Pa^{-1}] → Typical value for melts

$\Delta p \approx 20$ MPa $\Leftrightarrow$ $\Delta\rho/\rho_0 \approx 3\%$

FVM Discretization

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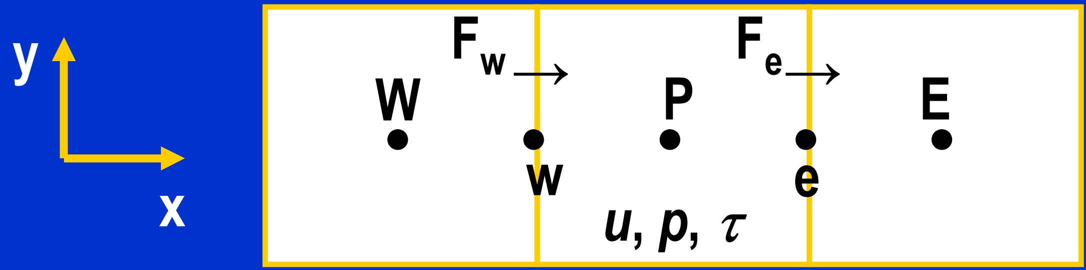

Mass as usual:
(1D for illustration)

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}\left(\rho u\right) = 0 \Leftrightarrow \frac{\rho_P^{n+1} V_P^{n+1} - \rho_P^n V_P^n}{\Delta t} + \left(F_e^{\,n+1} - F_w^{\,n+1}\right) = 0$$

$$F = \rho A u$$

Momentum as usual:
(1D for illustration)

$$a_P u_P = \sum a_F u_F + \left\{ A_P \Delta p_P + S \right\}$$

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n – previous time

A – cell face area

S – Source term

n+1 – new time (dropped)

V – Volume area

Pressure correction method

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Variations of pressure (p') affect both velocity (u') and density (ρ'):

- **Motion equation for face velocity:** ("east" face)

$$u_e = \frac{1}{a_P}\overline{\sum a_F u_F} + \overline{S} + \frac{1}{a_P} A_e \left(p_P - p_E\right) \Leftrightarrow$$

$$\Leftrightarrow u'_e = d_e \left(p'_P - p'_E\right)$$

- **Equation of state:**

$$\rho_e = \rho_0 + \rho_0 K_e \left(p_e - p_0\right) \Leftrightarrow$$

$$\Leftrightarrow \rho'_e = \rho_0 K_e p'_e$$

These corrections are applied to the "imperfect" mass flux F^* to obtain continuity satisfying fluxes F^{n+1}.

$$F^{n+1} = F^* + F' \cong \left(\rho^* A u^*\right) + A\left(\rho' u^* + \rho^* u'\right)$$

For the "east" face (central differences scheme for $p_e = \left(p_P + p_E\right)/2$):

$$F_e^{n+1} = F_e^* + \underbrace{A_e \rho_e^* d_e \left(p'_P - p'_E\right)}_{\text{usual term, no compressibility (diffusion like)}} + \underbrace{\frac{\rho_0 A_e u_e^* K_e}{2}\left(p'_P + p'_E\right)}_{\text{new term, due to compressibility (convection like)}}$$

Pressure correction equation

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Inserting into continuity equation and re-grouping:

$$a_P^p p_P' = \sum_F a_F^p p_F' + b^p$$

with $a_E^p = \rho_e{}^* A_e d_e - \left\{ \frac{1}{2} F_e{}^* K_e \rho_0 \Big/ \rho_e{}^* \right\}$

$$a_W^p = \rho_w{}^* A_w d_w + \left\{ \frac{1}{2} F_w{}^* K_w \rho_0 \Big/ \rho_w{}^* \right\}$$

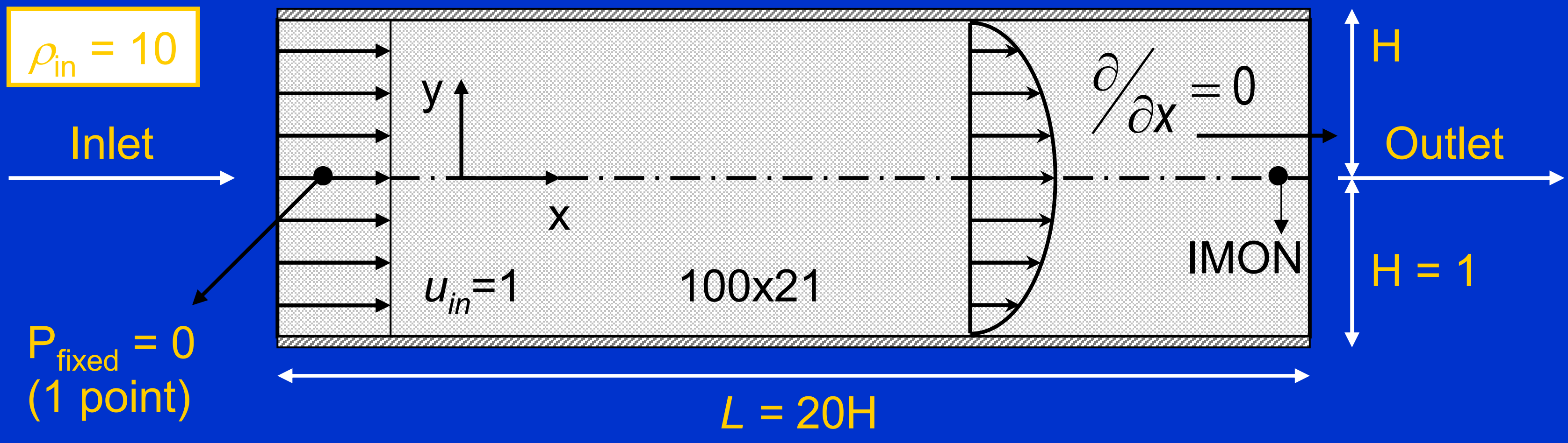
$$a_P^p = \sum a_F^p + \left\{ \frac{K_p V_p}{\Delta t} + \left(F_e{}^* K_e \rho_0 / \rho_e{}^* - F_w{}^* K_w \rho_0 / \rho_w{}^* + \ldots \right) \right\}$$

$$b^p = -\left[\underbrace{\frac{\rho_P^* V_P - \rho_P^n V_P^n}{\Delta t} + \left(F_e^* - F_w^* + \ldots \right)}_{=0 \text{ at convergence, when continuity is satisfied}} \right]$$

- Pressure equation is non symmetric: - coefficients now have convective influences;
  - New solver (BCG).

Flow domain and Boundary Conditions

1) Standard (as in incompressible - Q given):



$$Re = \frac{\rho u_{in} H}{\eta_0} = 10$$

2) p_{out} is given (instead of $\partial/\partial x = 0$)

$\rho_{in} = 10$ $\quad$ $p_{out} = 0$

$$\dot{M}_{in} = \rho_{in} A_{in} u_{in} = 10x2x1 = 20$$

3) ρ_{in} is variable

ρ_{in} = variable ⇔ $f(p_{in})$ $\quad$ $p_{out} = 0$

$$\dot{M}_{in} = \rho_{in} A_{in} u_{in} = \text{varies}$$

Results:

Incompressible *vs* Compressible flows (steady formulation)

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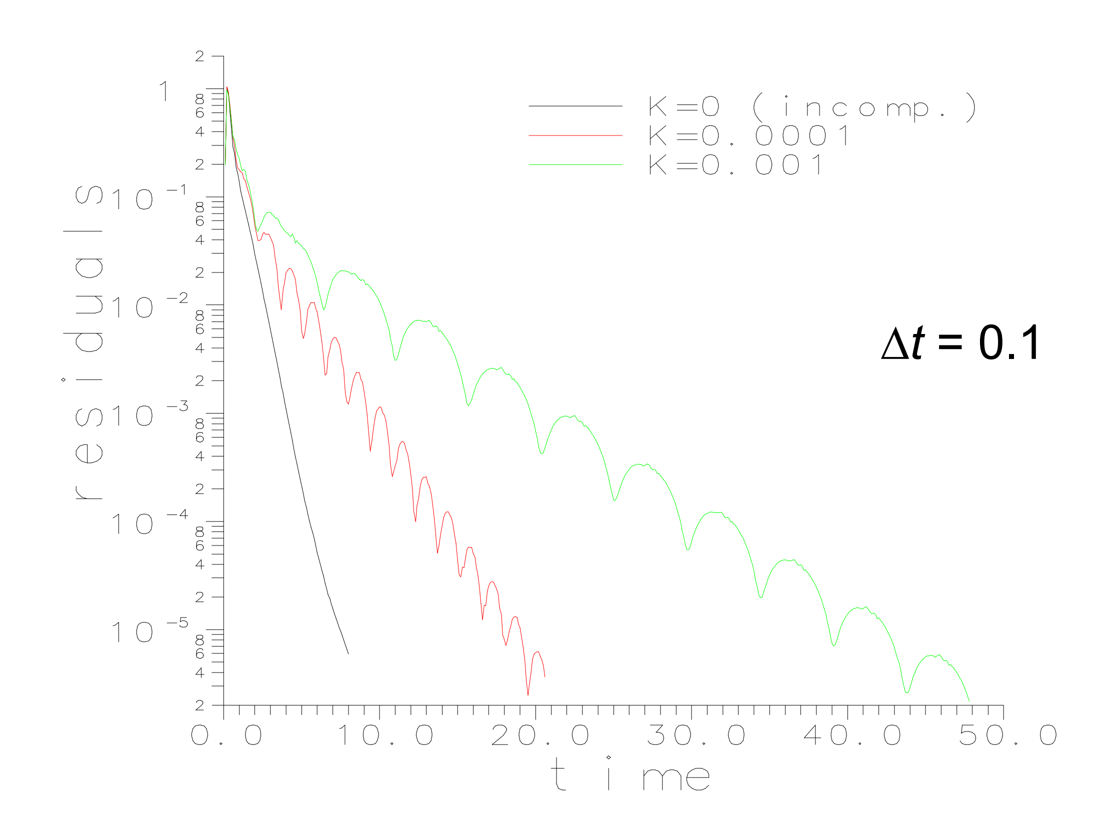

Simple test case: Channel flow with imposed uniform inlet velocity.

Boundary conditions: u_{in} and ρ_{in} are given => $\dot{M}_{in}$ fixed at outlet, and $\partial\phi / \partial x = 0$

- Even a small compressibility ($K \approx 10^{-4}$) affects the time-evolution of a channel flow.
- Weakly compressible solutions oscillate and more iterations are needed in order to achieve convergence with increasing K value.

Results: Compressible flow – theoretical *vs* numerical (steady formulation)

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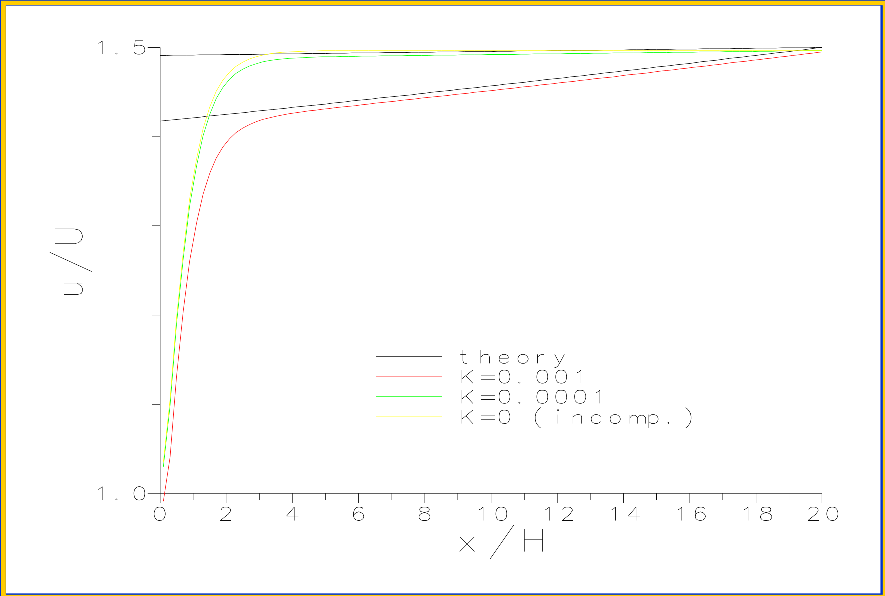
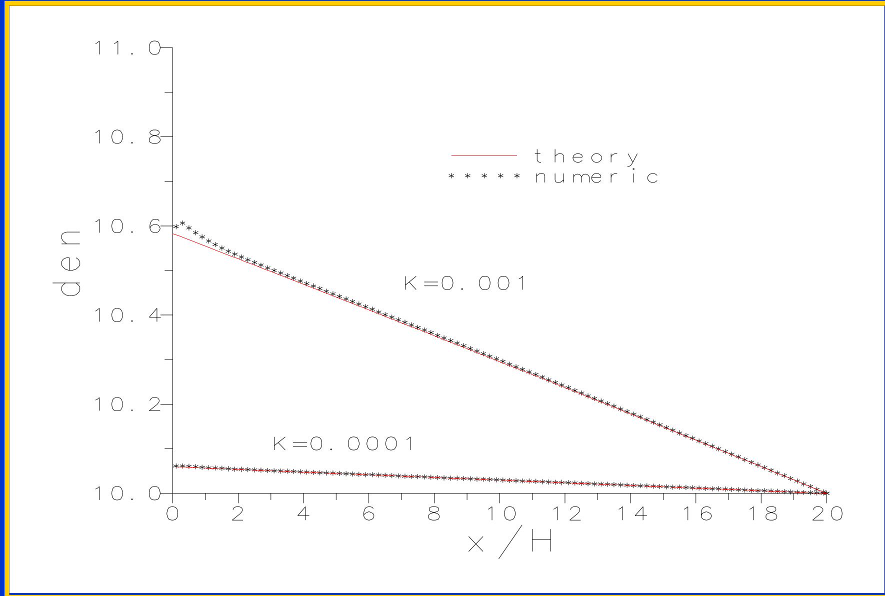
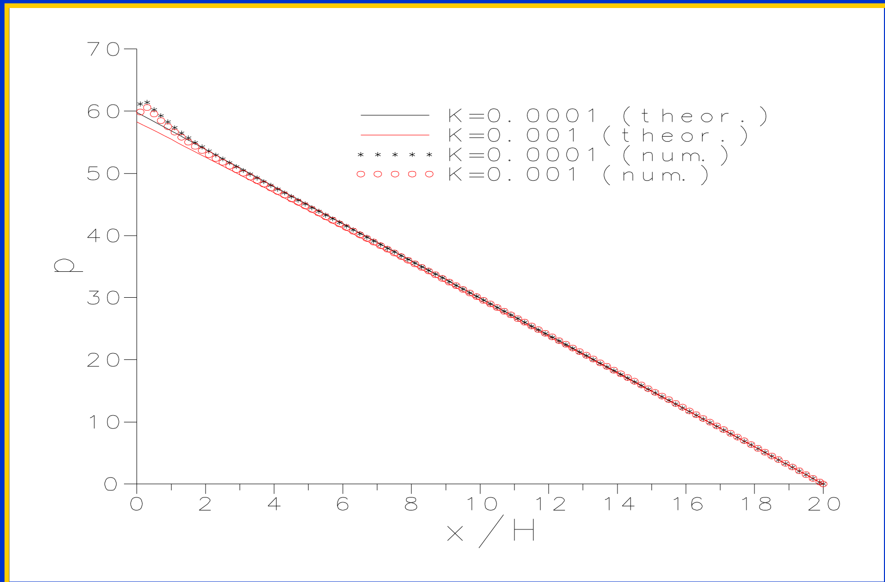




The theoretical solution is given in Georgiou & Crochet, J. Rheology 38(3) 639- (1994) .

The steady solution compares well with the theoretical solution, using two compressibility factors.



Results: Compressible flows – Boundary conditions comparison (steady formulation)

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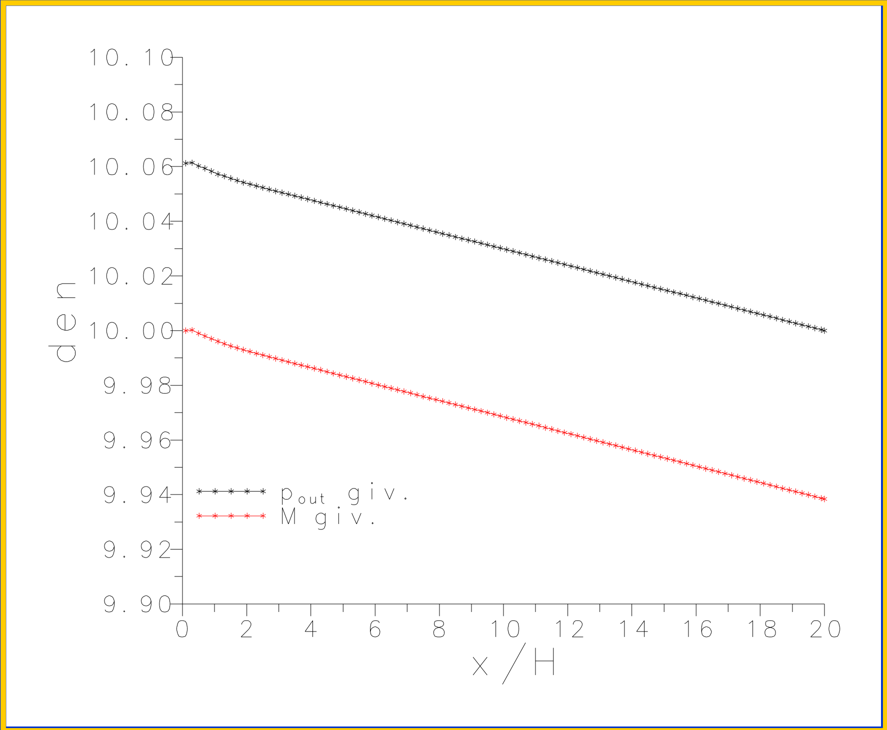

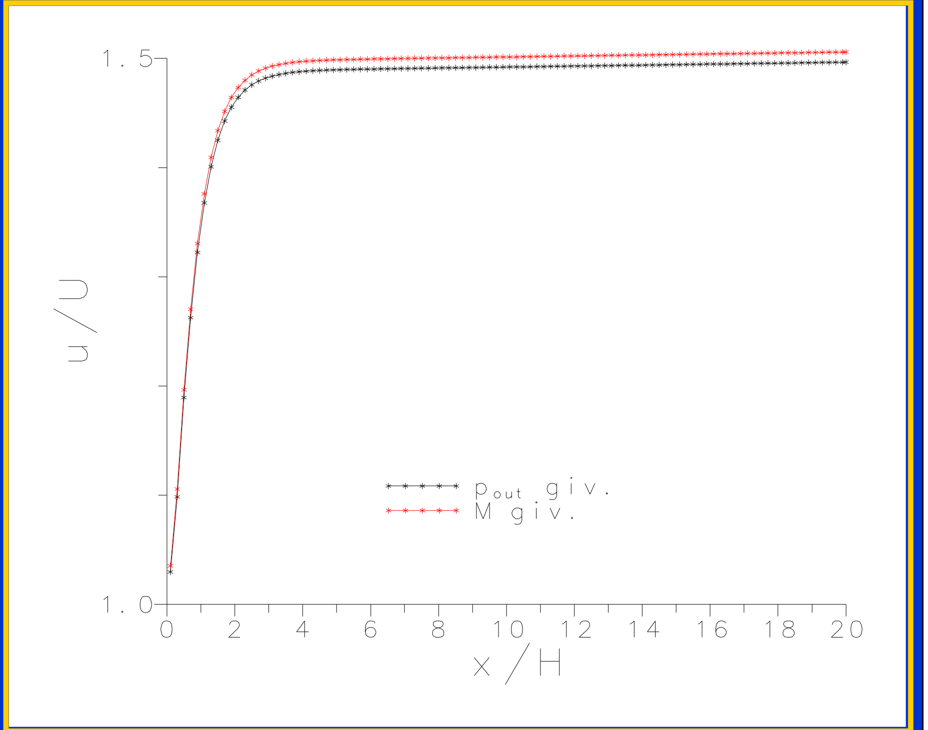

- With these boundary conditions, for steady calculations, the convergence behaviour remains essentially unchanged.
- The convergence rate, not shown here, is slightly affected by the choice of the BC.

Results: Compressible flows – Newtonian fluid (time-dependent formulation)

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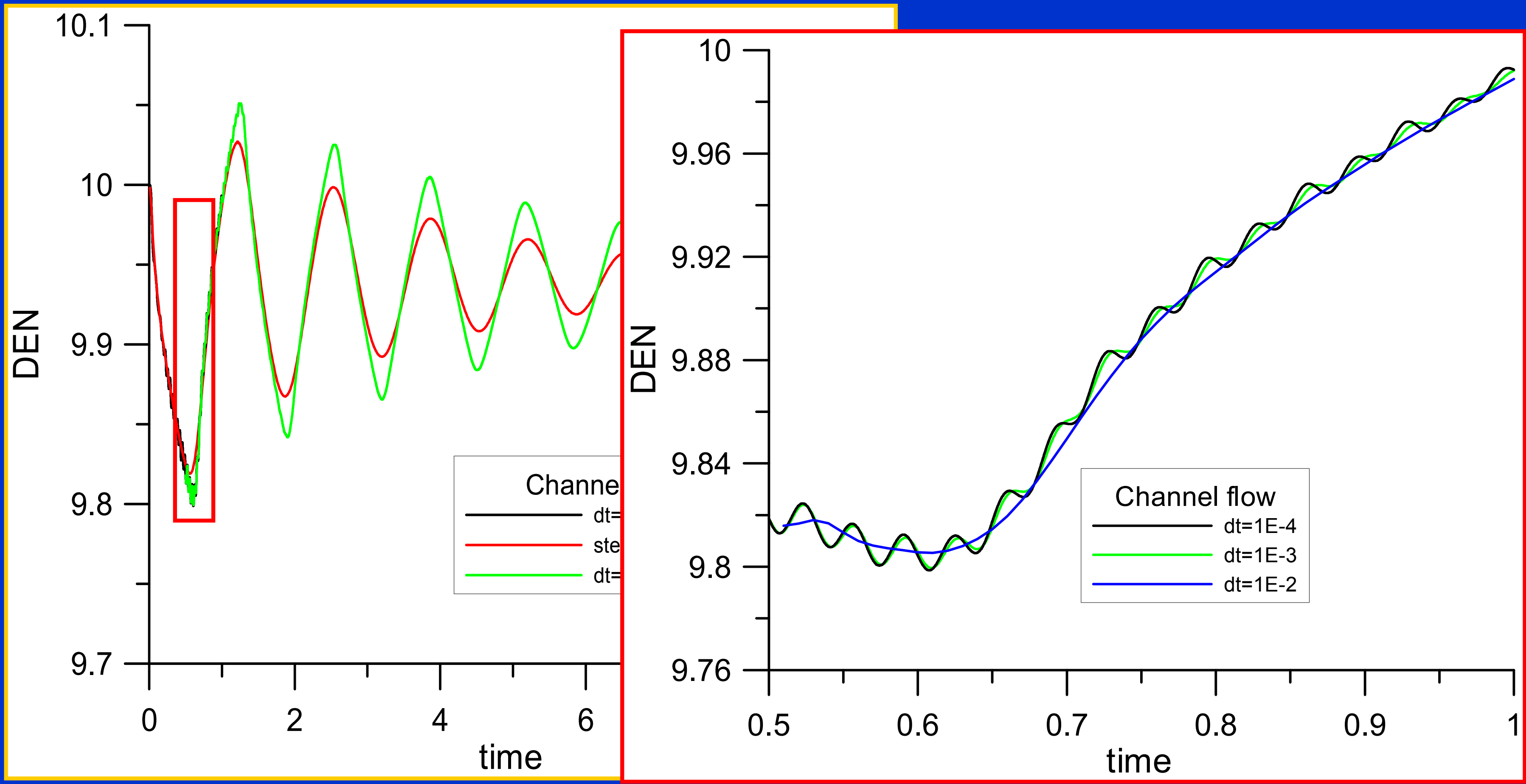

- Time-dependent calculation (Δt = 0.001) showing that the exact time evolution of the flow was captured andthe long-wave oscillations verified.
- Short-wave oscillations are also present, requiring small time-steps.

Results: Compressible flows –
Newtonian *vs* viscoelastic case (time-dependent formulation)

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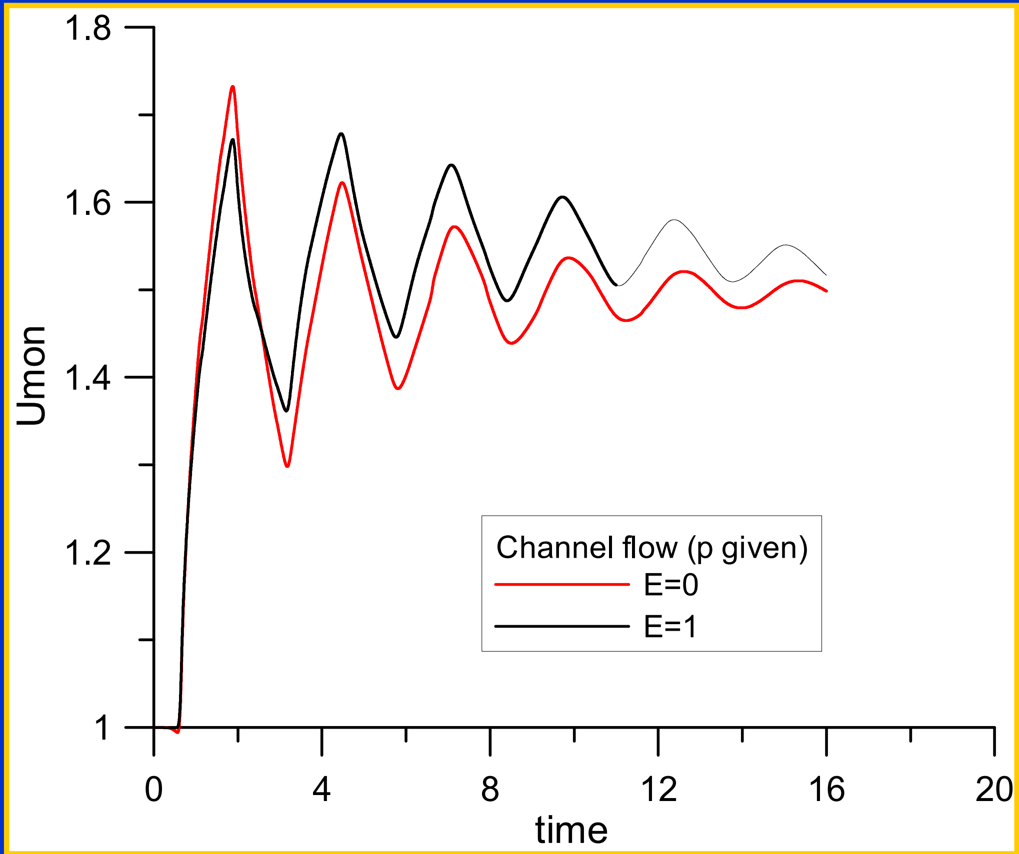

FENE-MCR fluid:
- $L^2 = 100$;
- $\beta = 0.5$;
- $E = 1$ (We = 10).

- The oscillating nature of flow development is present in the viscoelastic case.
- Viscoelasticity does not change significantly time evolution, although magnitude and period are somewhat different.

Heading towards…

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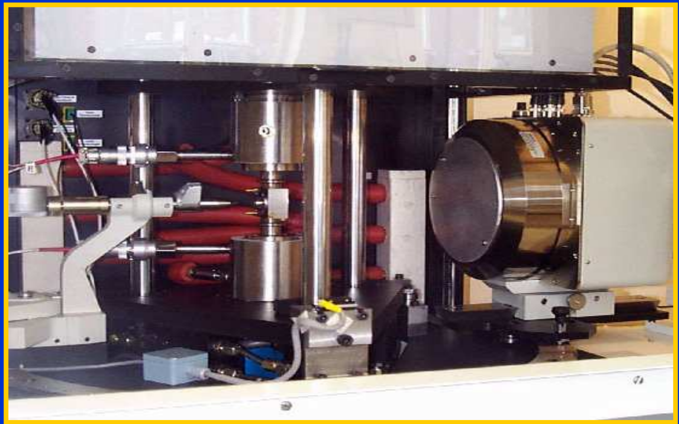
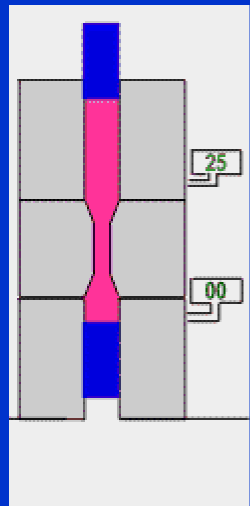
- Application of this formulation to moving meshes:





In order to simulate the multipass rheometer (MPR) in Cambridge.

Aknowledgments

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