Computing Viscoelastic Fluid Flows at High Weissenberg Number

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Outline

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What is a viscoelastic fluid?

from *The Institute of Non-Newtonian Fluid Mechanics, University of Wales*

Characteristics of Viscoelastic Fluids

- Viscoelastic materials have properties between those of elastic materials and viscous fluids
- Additional information (constitutive law) is required to describe the internal stresses on fluid particles
- The effects of fluid **memory** influence the flow
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Mathematical Model

If V is an arbitrary volume within the domain Ω,

$$\frac{d}{dt}\int_V \rho\mathbf{u}\, dV = \int_V \mathbf{f}\, dV + \int_{\partial V} \mathbf{T}\cdot\mathbf{n}\, dS \quad \text{(momentum)}$$

$$\frac{d}{dt}\int_V \rho\, dV = -\int_{\partial V} \rho\mathbf{u}\cdot\mathbf{n}\, dS \quad \text{(mass)}$$

Assuming the fluid is incompressible and has constant density, the momentum and mass equations reduce to

$$\frac{\partial\mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} = \mathbf{f} + \nabla\cdot\mathbf{T} \quad \text{in } \Omega\,,$$

$$\nabla\cdot\mathbf{u} = 0 \quad \text{in } \Omega\,.$$

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The Stress Tensor

$$\mathbf{T} = -p\mathbf{I} + \boldsymbol{\sigma}_e,$$

where $\boldsymbol{\sigma}_e$ is the extra stress tensor.

Newtonian Fluid

Extra stress tensor $\boldsymbol{\sigma}_e$ is proportional to the deformation tensor $D(\mathbf{u})$:

$$\boldsymbol{\sigma}_e = \boldsymbol{\sigma}_N = \mu D(\mathbf{u}) = \mu \frac{1}{2}\left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right).$$

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Extra stress is more complicated - in many cases $\boldsymbol{\sigma}_e \neq F(\mathbf{u})$

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Viscoelastic Fluid Flow Constitutive Models

Power Law Model: $\boldsymbol{\sigma}_e = \left(\kappa_0 + \kappa_1 |\nabla \mathbf{u}|^{\beta-2}\right) D(\mathbf{u}),\ 1 < \beta \leq 2$

Carreau Model: $\boldsymbol{\sigma}_e = \left(\kappa_0 + \kappa_1 (1 + |\nabla \mathbf{u}|^2)^{(\beta-2)/2}\right) D(\mathbf{u}),\ 1 < \beta \leq 2$

Objective Time Derivative:

$$\frac{\hat{\partial}\boldsymbol{\sigma}}{\partial t} = \frac{\partial \boldsymbol{\sigma}}{\partial t} + \mathbf{u} \cdot \nabla \boldsymbol{\sigma} + g_a(\boldsymbol{\sigma}, \nabla \mathbf{u}), \quad a \in [-1, 1]$$

where

$$g_a(\boldsymbol{\sigma}, \nabla \mathbf{u}) := \frac{1-a}{2}(\boldsymbol{\sigma} \nabla \mathbf{u} + \nabla \mathbf{u}^T \boldsymbol{\sigma}) - \frac{1+a}{2}(\nabla \mathbf{u}\, \boldsymbol{\sigma} + \boldsymbol{\sigma} \nabla \mathbf{u}^T).$$

Johnson-Segalman Model: $(\boldsymbol{\sigma}_e = \boldsymbol{\sigma}_N + \boldsymbol{\sigma}_V)$ $\quad \boldsymbol{\sigma}_V + \lambda \frac{\hat{\partial}\boldsymbol{\sigma}_V}{\partial t} - 2\alpha D(\mathbf{u}) = 0$

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Johnson-Segalman Model

(Re: Reynolds number, λ: Weissenberg number)

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\begin{aligned}
\mathrm{Re}\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) + \nabla p - 2(1-\alpha)\,\nabla\cdot D(\mathbf{u}) - \nabla\cdot\boldsymbol{\sigma} &= \mathbf{f} \ \text{ in } \Omega, \\
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\nabla\cdot\mathbf{u} &= 0 \ \text{ in } \Omega, \\
\mathbf{u} &= \mathbf{u}_\Gamma \ \text{ on } \Gamma, \\
\boldsymbol{\sigma} &= \boldsymbol{\sigma}_\Gamma \ \text{ on } \Gamma_{in}, \\
\mathbf{u}(\mathbf{x}, 0) &= \mathbf{u}_0 \ \text{ in } \Omega, \\
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Theoretical Results, differential-type constitutive equations

If $\mathbf{f}$ is sufficiently regular and small, then for some $0 \leq \lambda \leq \lambda_0$ the steady-state problem admits a unique bounded solution $(\sigma, \mathbf{u}, p) \in \mathbf{H}^2(\Omega) \times \mathbf{H}^3(\Omega) \times H^2(\Omega)$ (Renardy 1985), (Guillopé and Saut 1990), (Fernández-Cara, Guillen, and Ortega 2001)

In contrast to Navier-Stokes, well-posedness for general models in viscoelasticity is still not well understood. Results which are known (Renardy 2000):

1. for initial value problems, solutions have been shown to exist locally in time
2. global existence of solutions which are small perturbations of the rest state (slow or creeping flow)
3. for steady-state problems, existence of solutions which are small perturbations of the analogous Newtonian case

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FEM Approximation - DG Method

- Velocity and pressure approximation: Taylor-Hood elements $(\mathbf{u}^h, p^h) \in \mathbf{X}^h \times Q^h$ for $(\mathbf{u}, p)$, satisfying

$$\inf_{0 \neq q^h \in S^h} \sup_{0 \neq \mathbf{v}^h \in \mathbf{X}^h} \frac{(q^h, \nabla \cdot \mathbf{v}^h)}{\|\mathbf{v}^h\|_1 \|q^h\|_0} \geq C$$

- Stress approximation: discontinuous piecewise linears $\boldsymbol{\sigma}^h \in \boldsymbol{\Sigma}^h$ for $\boldsymbol{\sigma}$
- Define

$$< \sigma^{\pm}, \tau^{\pm} >_{h,\mathbf{u}} := \sum_{K \in T_h} \int_{\partial K^-(\mathbf{u})} (\sigma^{\pm}(\mathbf{u}) : \tau^{\pm}(\mathbf{u})) |\mathbf{n} \cdot \mathbf{u}| \, ds$$

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Discrete Problem

Find $(\boldsymbol{\sigma}^h, \mathbf{u}^h, p^h) \in \boldsymbol{\Sigma}^h \times \mathbf{X}^h \times Q^h$ *such that*

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(\boldsymbol{\sigma}^h, D(\mathbf{v}^h)) + 2(1-\alpha)\,(D(\mathbf{u}^h), D(\mathbf{v}^h)) - (p^h, \nabla \cdot \mathbf{v}^h) &= (\mathbf{f}, \mathbf{v}^h) \quad \forall \mathbf{v}^h \in \mathbf{X}^h, \\
(q^h, \nabla \cdot \mathbf{u}^h) &= 0 \quad \forall q^h \in Q^h.
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Theorem

Existence, uniqueness, and

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\begin{aligned}
\|\boldsymbol{\sigma} - \boldsymbol{\sigma}^h\|_0 + \|\nabla(\mathbf{u} - \mathbf{u}^h)\|_0 &\le Ch^{3/2}, \\
\|p - p^h\|_0 &\le Ch^{3/2}
\end{aligned}
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shown by Baranger and Sandri 1992 for "small enough" $\boldsymbol{\sigma}, \mathbf{u}, p$.

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Nonlinear Solution Approach

Let $\underline{\mathbf{u}} := (\boldsymbol{\sigma}^h, \mathbf{u}^h, p^h)$, $\underline{\mathbf{v}} := (\boldsymbol{\tau}^h, \mathbf{v}^h, q^h) \in \boldsymbol{\Sigma}^h \times \mathbf{X}^h \times Q^h = \boldsymbol{\Pi}^h$ and

$$A(\underline{\mathbf{u}}, \underline{\mathbf{v}}) := (\boldsymbol{\sigma}^h, \boldsymbol{\tau}^h) - 2\alpha(D(\mathbf{u}^h), \boldsymbol{\tau}^h) + (\boldsymbol{\sigma}^h, D(\mathbf{v}^h)) + 2(1-\alpha)\,(D(\mathbf{u}^h), D(\mathbf{v}^h)) - (p^h, \nabla\cdot\mathbf{v}^h) + (q^h, \nabla\cdot\mathbf{u}^h) - (\mathbf{f}, \mathbf{v}^h)$$

and define $\mathbf{G}$ by

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Then the equation $\mathbf{G}(\underline{\mathbf{u}}) = 0$ is solved via Newton Iteration: given $\underline{\mathbf{u}}_0$, for $i = 0, 1, 2, \ldots$

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until $\|\underline{\mathbf{u}}_{i+1} - \underline{\mathbf{u}}_i\| < tol$.

Nonlinear Solution Approach

Let $\underline{\mathbf{u}} := (\boldsymbol{\sigma}^h, \mathbf{u}^h, p^h)$, $\underline{\mathbf{v}} := (\boldsymbol{\tau}^h, \mathbf{v}^h, q^h) \in \boldsymbol{\Sigma}^h \times \mathbf{X}^h \times Q^h = \boldsymbol{\Pi}^h$ and

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Difficulties in Numerical Simulations

- Mixed FEM requires a large number of unknowns
- The hyperbolic nature of the constitutive equation requires upwinding and stabilization techniques, such as SUPG, DG, or EVSS methods
- The High Weissenberg Number Problem:
  - Computations become more difficult for increasing values of λ
  - For many problems, there is a critical value λ^* such that nonlinear solvers fail for $\lambda > \lambda^*$
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Outline

Some Numerical Approaches to the HWNP

- Numerical continuation methods (embedding methods) are widely used to compute solution manifolds of a system of equations $\mathbf{F}(\mathbf{y}, \gamma) = \mathbf{0}$ (one or more parameters γ).

- Main idea: trace out solution curves (surfaces) in the $\gamma\mathbf{y}$-space using predictor-corrector procedure

- Main results: Keller, Rheinboldt, Allgower and Georg

- Applications to Navier-Stokes: Gunzburger and Peterson, Carey and Krishnan, de Almeida and Derby

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Continuation in λ

Let $\mathbf{G}(\underline{\mathbf{u}}, \lambda) = \mathbf{G}(\underline{\mathbf{u}})$. Using λ as continuation parameter, given a solution at $(\underline{\mathbf{u}}_0, \lambda_0)$

1. Compute tangent to curve at $(\underline{\mathbf{u}}_0, \lambda_0)$ by solving

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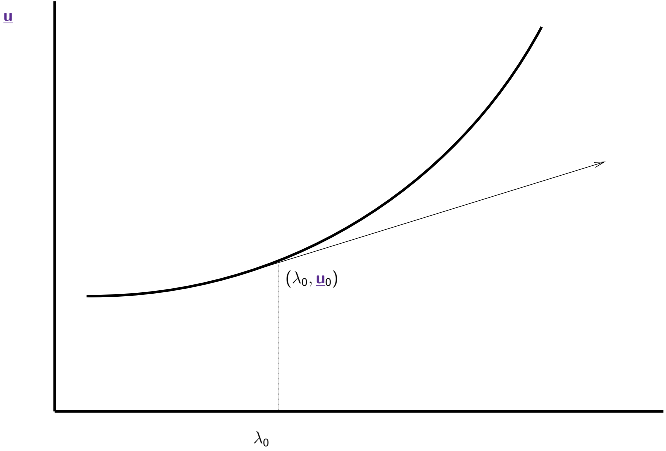
Like simple continuation, method results in same procedure as standard Newton iteration with different initial data.

Illustration of the Method



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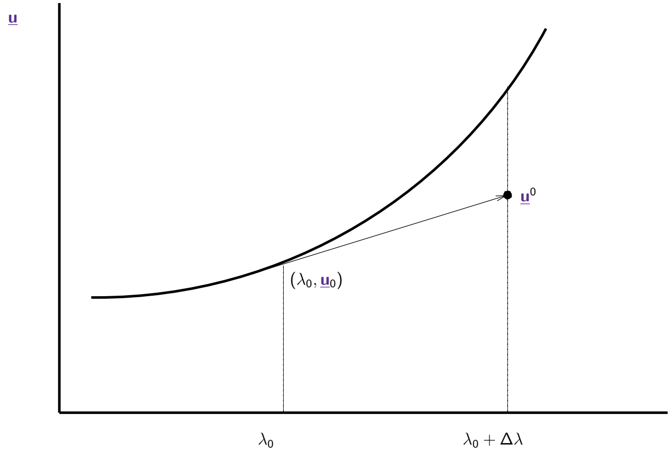

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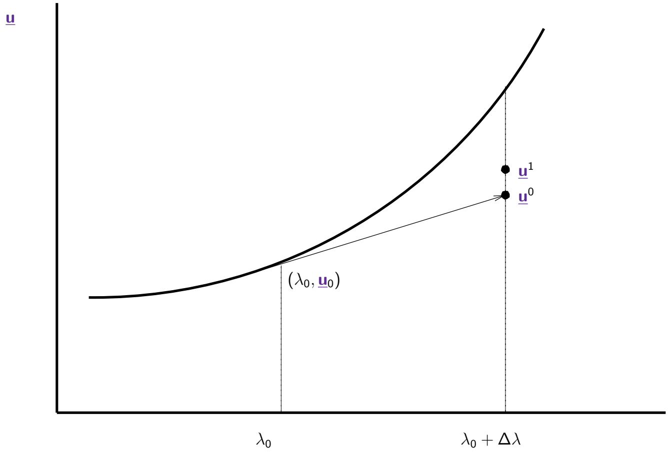

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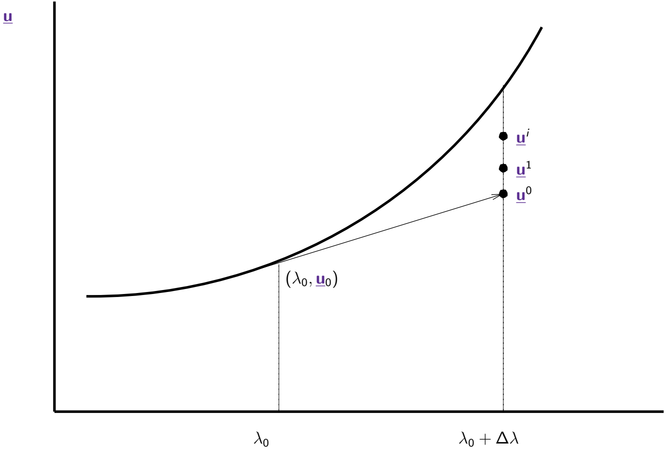

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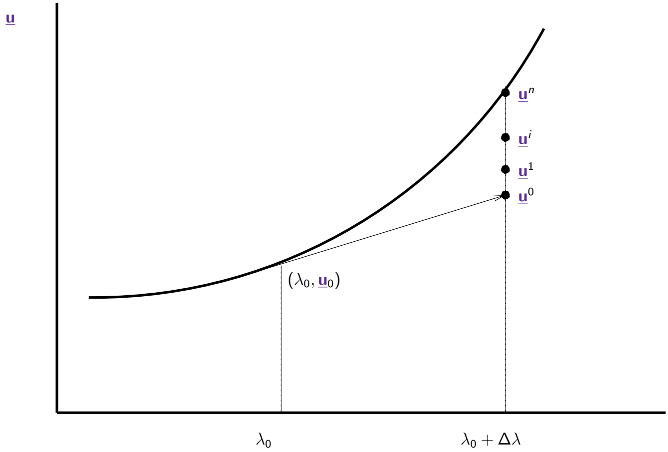

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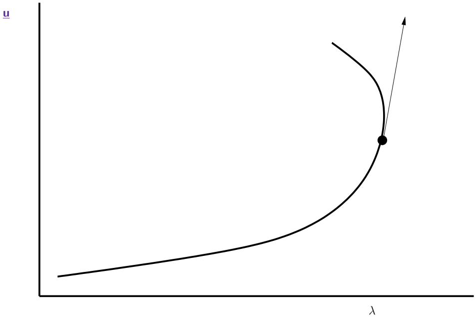

Outline

Reparametrize the Solution Curve

- Treat $\underline{\mathbf{u}}(s)$ and $\lambda(s)$ both as functions of an arclength-like parameter
- Augment $\mathbf{G}(\underline{\mathbf{u}}(s), \lambda(s)) = \mathbf{0}$ with a pseudo-arclength constraint $N(\underline{\mathbf{u}}(s), \lambda(s), s) = 0$

1. Compute tangent $(\dot{\underline{\mathbf{u}}}_0, \dot{\lambda}_0)$ to curve at $(\underline{\mathbf{u}}_0, \lambda_0)$
2. Form predictor

$$\underline{\mathbf{u}}^0 = \underline{\mathbf{u}}_0 + (\Delta s)\dot{\underline{\mathbf{u}}}_0, \qquad \lambda^0 = \lambda_0 + (\Delta s)\dot{\lambda}_0$$

3. Solve nonlinear system $[\mathbf{G}(\underline{\mathbf{u}}, \lambda), N(\underline{\mathbf{u}}, \lambda, s)]^T = \mathbf{0}$ by Newton iteration:

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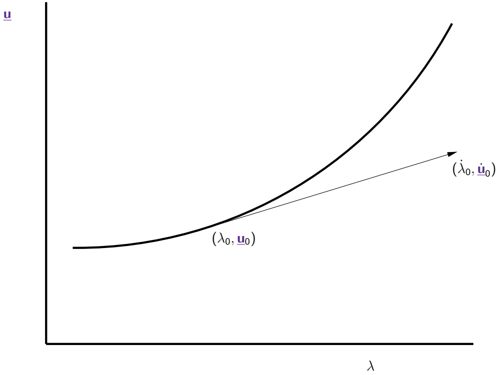

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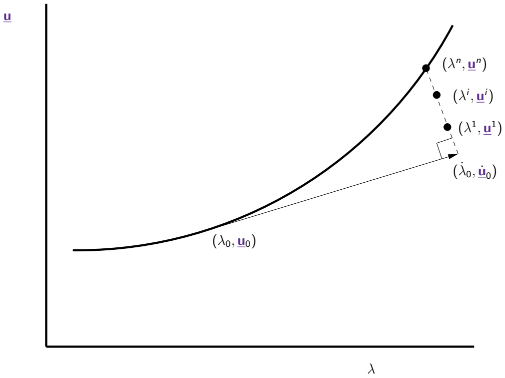

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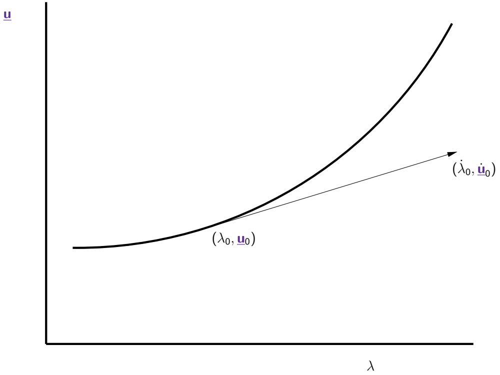

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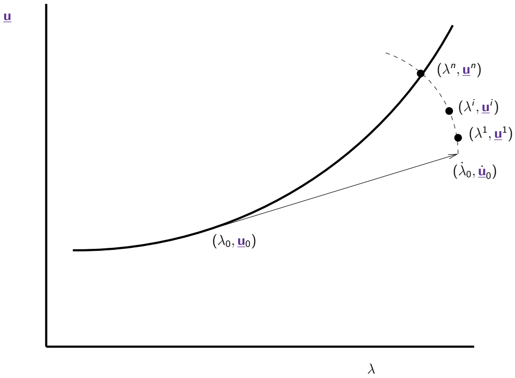

Outline

Four-to-One Contraction Problem

Implemented using `FreeFem++` finite element framework, UMFPACK solver

- Planar contraction: $(\alpha = 8/9)$

- Inflow boundary conditions for velocity and stress
- Outflow boundary conditions for velocity
- Computations done on two nonuniform meshes:

$$\text{M1} \xrightarrow{h/2} \text{M2}$$

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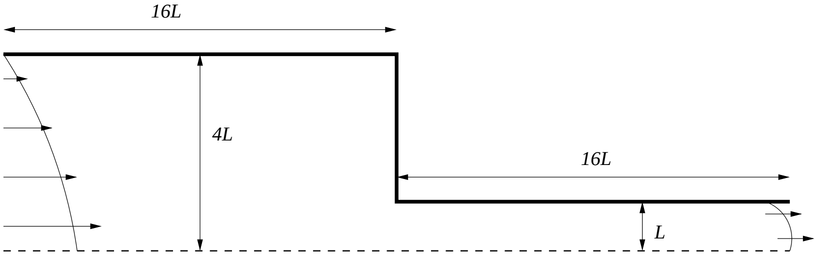

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- Computations done on two nonuniform meshes:

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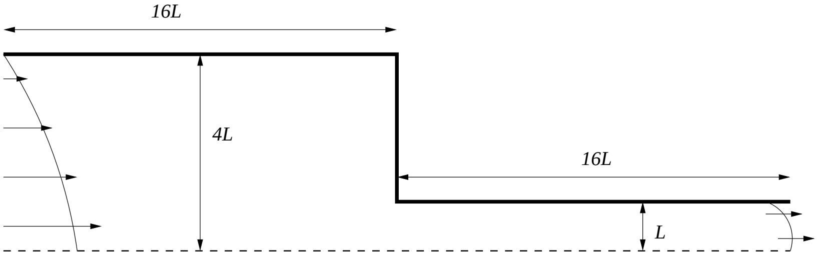
Four-to-One Contraction Problem

Implemented using `FreeFem++` finite element framework, UMFPACK solver

- Planar contraction: $(\alpha = 8/9)$



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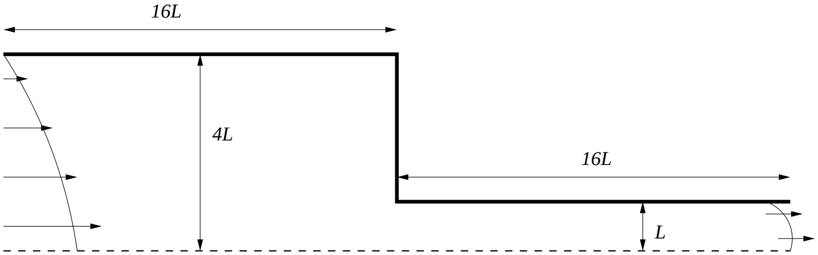

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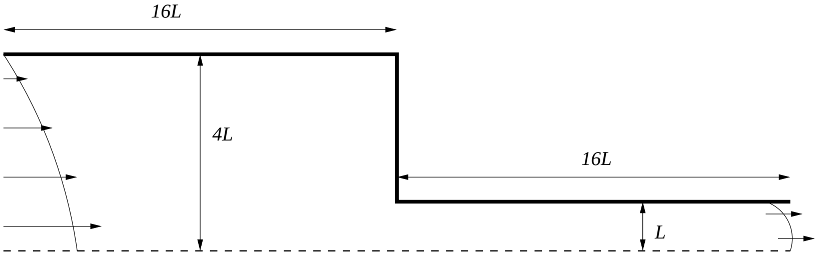

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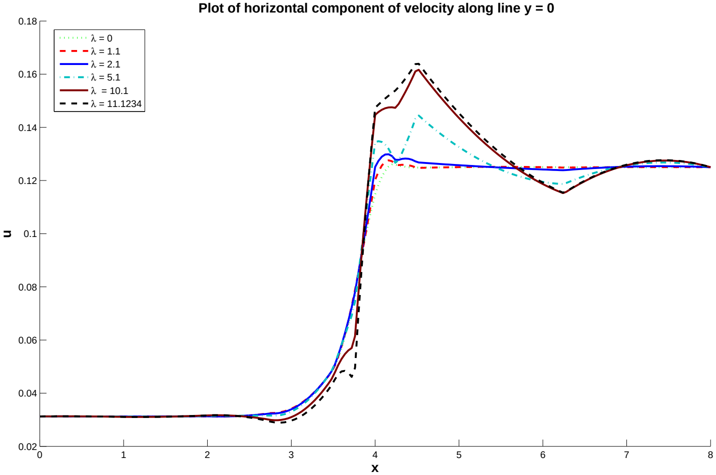
Outline

High Weissenberg Number Limits

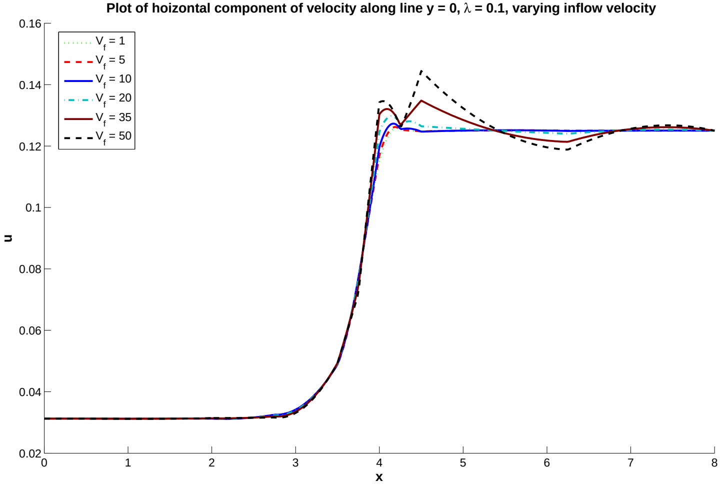
For the different methods, the maximum λ computed

Mesh	a	Simple Continuation	Natural Continuation	Pseudo-arclength Continuation (N_2)
M1	1.0	11.1279	11.1279	11.1291
	0.0	18.1992	18.2187	18.3423
	-1.0	8.904	8.9399	8.9559
M2	1.0	9.337	9.346	9.3466
	0.0	9.0184	9.0234	9.1348
	-1.0	9.1563	9.3007	9.1892

Solutions for increasing λ

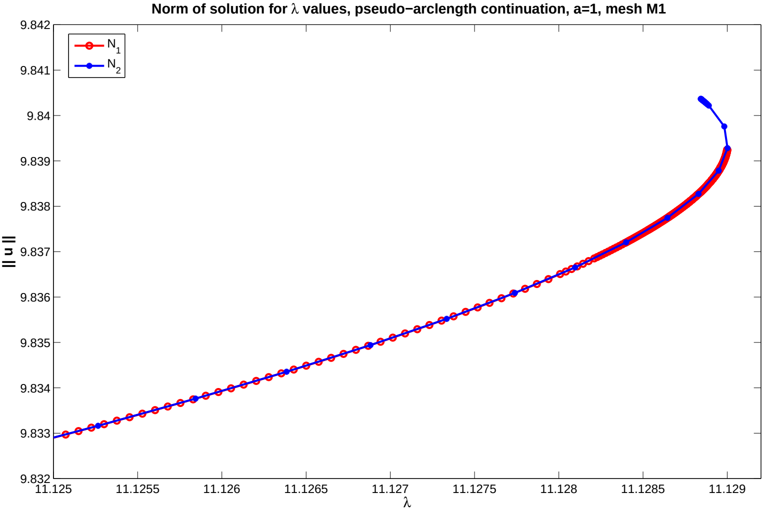


Solutions for increasing velocity



Outline

Behavior at High λ for N_1, N_2



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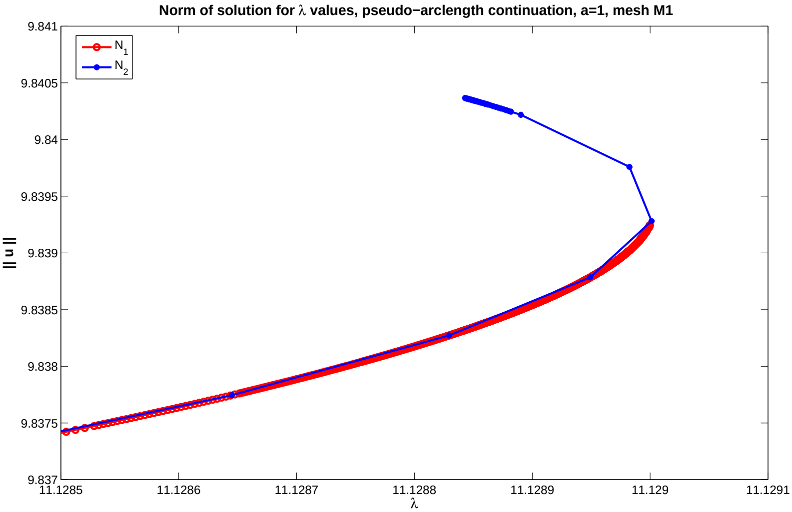
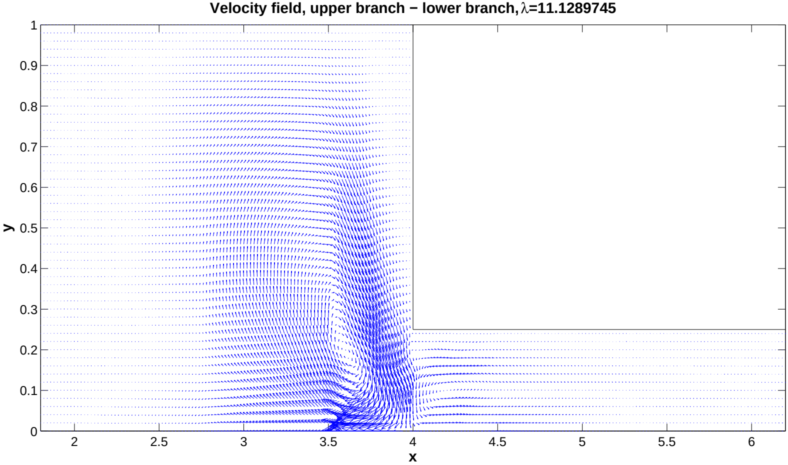


Solutions on an Unstable Branch?



Some Other Results

- So far, the turning point behavior has not been seen under mesh refinement or for different choices of a
- Variations of arclength constraints are being examined

$$N_{2,\theta}(\underline{\mathbf{u}}, \lambda, s) \equiv \theta \|\underline{\mathbf{u}}^i - \underline{\mathbf{u}}_0\|^2 + (1-\theta)|\lambda^i - \lambda_0|^2 - \Delta s^2 = 0$$

- Fewer steps and steplength reductions are seen in pseudo-arclength continuation. Example: $a = 1$, mesh M1

Method	max λ	Total # of steps	# of steplength reductions
Simple	11.1279	28	25
Natural	11.1279	28	25
Pseudo-arclength	11.1291	11	7

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Conclusions and Future Work

- Continuation methods provide efficient ways to compute solutions for high Weissenberg number.
- However, limitations still exist as computations exhibit a critical value.
- More investigations need to be performed at large λ to see if we can make any inferences about the discrete problem.
- Apply these methods to additional benchmark problems (e.g. flow around a cylinder) and investigate solution behavior for large λ.
- Analyze further aspects of continuation algorithms for viscoelastic fluids (arclength constraints, steplength selection, multiparameter continuation).

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