

Numerical Schemes for Materials with Fine Scale Structure

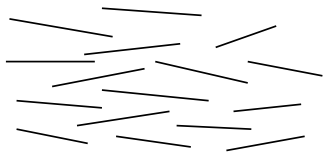
Noel Walkington

Department of Mathematical Sciences
Carnegie Mellon University
Pittsburgh, PA, USA

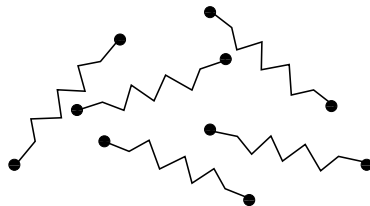
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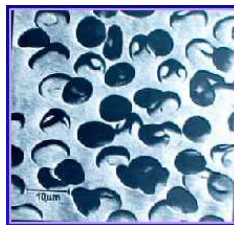
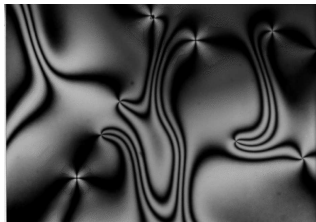
Fluids Exhibiting Elastic Response



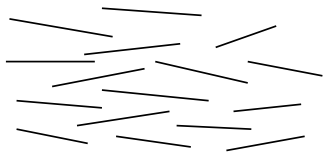
Nematic Liquid Crystal



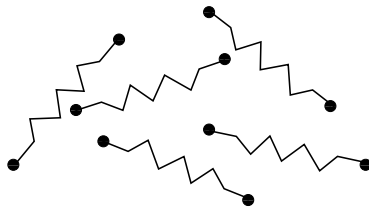
Oldroyd-B Fluid



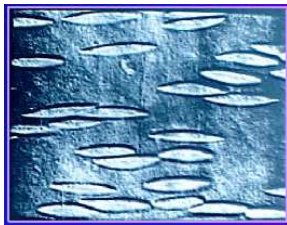
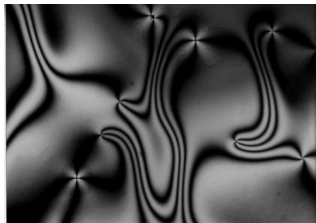
Fluids Exhibiting Elastic Response



Nematic Liquid Crystal



Oldroyd-B Fluid



Numerical PDE

Lax Richtmyer Equivalence Theorem: *A numerical scheme for a linear pde converges if and only if it is*

- ▶ *Consistent and*
- ▶ *Stable.*

Nonlinear pde's additionally require

- ▶ *Compactness ...*

Galerkin Schemes:

- ▶ **Consistency** follows directly from the discrete weak statement.
- ▶ **Compactness** is typically inherited from the continuous problem.
- ▶ **Stability** frequently problematic (insufficient test functions).

Ericksen Leslie Equations

Linear Momentum Equation: $\operatorname{div}(v) = 0$

$$\rho \dot{v} - \operatorname{div}(-pl + \mu D(v) + T_v + T_e) = \rho f$$

Angular Momentum Equation: $|n| = 1$

$$\rho \bar{r}^2 \ddot{n} + g_v + g_e - \operatorname{div}(C_e) + \lambda n = \rho g$$

Notation:

- ▶ $\dot{v} = v_t + (v \cdot \nabla)v$
- ▶ $\operatorname{div}(T)_i = \sum_j \partial T_{ij} / \partial x_j$
- ▶ $(\nabla v)_{ij} = \partial v_i / \partial x_j$
- ▶ $D(v) = (1/2)(\nabla v + (\nabla v)^T)$
- ▶ $W(v) = (1/2)(\nabla v - (\nabla v)^T)$

Ericksen Leslie Equations

Linear Momentum Equation: $\operatorname{div}(v) = 0$

$$\rho \dot{v} - \operatorname{div}(-pI + \mu D(v) + T_v + T_e) = \rho f$$

Angular Momentum Equation: $|n| = 1$

$$\rho \bar{r}^2 \ddot{n} + g_v + g_e - \operatorname{div}(C_e) + \lambda n = \rho g$$

Elastic Terms: Strain energy $\mathcal{W}(n, \nabla n)$

$$T_e = \mathcal{W}I - (\nabla n)^\top \left[\frac{\partial \mathcal{W}}{\partial \nabla n} \right] \quad g_e = \left(\frac{\partial \mathcal{W}}{\partial n} \right) \quad C_e = \left[\frac{\partial \mathcal{W}}{\partial \nabla n} \right]$$

Dissipative Terms: Raleighian $\mathcal{R}(n, \dot{n}, \nabla v)$ (Parodi)

$$g_v = \left(\frac{\partial \mathcal{R}}{\partial \dot{n}} \right) \quad T_v = \left[\frac{\partial \mathcal{R}}{\partial \nabla v} \right]$$

Ericksen Leslie Equations

Linear Momentum Equation: $\operatorname{div}(v) = 0$

$$\rho \dot{v} - \operatorname{div}(-pI + \mu D(v) + T_v + T_e) = \rho f$$

Angular Momentum Equation: $|n| = 1$

$$\rho \bar{r}^2 \ddot{n} + g_v + g_e - \operatorname{div}(C_e) + \lambda n = \rho g$$

Energy Estimate:

- ▶ Multiply linear momentum equation by v
- ▶ Multiply the angular momentum equation by $\dot{n} \equiv n_t + (v \cdot \nabla)n$
- ▶ Use the identity $\operatorname{div}(T_e) = (\nabla n)^\top (g_e - \operatorname{div}(C_e))$

$$\begin{aligned} & \frac{d}{dt} \int_{\Omega} \{ (\rho/2)(|v|^2 + |\bar{r}\dot{n}|^2) + \mathcal{W} \} \\ & + \int_{\Omega} \{ \mu |D(v)|^2 + (T_v, \nabla v) + (g_v, \dot{n}) \} = \int_{\Omega} (\rho f, v) + (\rho g, \dot{n}) \end{aligned}$$

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Problems: If $n_h \in \mathbb{N}_h \subset H^1(\Omega)$ (Lagrange elements)

- ▶ $\dot{n}_h = n_{ht} + (v_h \cdot \nabla)n_h \notin \mathbb{N}_h$
- ▶ $\operatorname{div}(C_e) = \operatorname{div}([\partial \mathcal{W} / \partial \nabla n])$ and $\operatorname{div}(T_e)$ are not defined for $n_h \in H^1(\Omega)$

Oldroyd-B Fluid: Classical Statement

Linear Momentum: $\operatorname{div}(\boldsymbol{v}) = 0$

$$\rho \dot{\boldsymbol{v}} - \operatorname{div} \left(-p \boldsymbol{I} + 2\mu_s D(\boldsymbol{v}) + \boldsymbol{T}_e \right) = \rho \boldsymbol{f}$$

Elastic Stress: $\boldsymbol{T}_e = \boldsymbol{T}_e^\top$

$$\dot{\boldsymbol{T}}_e - (\nabla \boldsymbol{v}) \boldsymbol{T}_e - \boldsymbol{T}_e (\nabla \boldsymbol{v})^\top + (1/We) \boldsymbol{T}_e = 2(\mu_p/We) D(\boldsymbol{v})$$

Notation:

- ▶ $(\nabla \boldsymbol{v})_{ij} = \frac{\partial v_i}{\partial x_j}$
- ▶ $D(\boldsymbol{v}) = (1/2) ((\nabla \boldsymbol{v}) + (\nabla \boldsymbol{v})^\top)$
- ▶ $\dot{\boldsymbol{T}} = \boldsymbol{T}_t + (\boldsymbol{v} \cdot \nabla) \boldsymbol{T}$

Oldroyd-B Fluid: Classical Statement

Linear Momentum: $\operatorname{div}(\boldsymbol{v}) = 0$

$$\rho \dot{\boldsymbol{v}} - \operatorname{div} \left(-p \boldsymbol{I} + 2\mu_s D(\boldsymbol{v}) + \boldsymbol{T}_e \right) = \rho \boldsymbol{f}$$

Conformation Tensor: $\boldsymbol{B} = (\textcolor{red}{We}/\mu_p) \boldsymbol{T}_e + \boldsymbol{I}$ is SPD

$$\dot{\boldsymbol{B}} - (\nabla \boldsymbol{v}) \boldsymbol{B} - \boldsymbol{B} (\nabla \boldsymbol{v})^\top + (1/\textcolor{red}{We}) \boldsymbol{B} = (1/\textcolor{red}{We}) \boldsymbol{I}$$

Classical Energy Estimate:

- ▶ Multiply the linear momentum equation by $\boldsymbol{v}$
- ▶ Take the trace of the equation for $\boldsymbol{B}$
- ▶ Take the dot product of the equation for $\boldsymbol{B}$ with $\boldsymbol{B}^{-1}$

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} (1/2) \left(\rho |\boldsymbol{v}|^2 + (\mu_p/\textcolor{red}{We}) (\operatorname{tr}(\boldsymbol{B} - \boldsymbol{I}) - \ln(\det(\boldsymbol{B}))) \right) \\ + \int_{\Omega} 2\mu_s |D(\boldsymbol{v})|^2 + (\mu_p/\textcolor{red}{We}^2) \operatorname{tr}(\boldsymbol{B} - 2\boldsymbol{I} + \boldsymbol{B}^{-1}) = \int_{\Omega} (\rho \boldsymbol{f} \cdot \boldsymbol{v}) \end{aligned}$$

Oldroyd-B Fluid: Classical Statement

Linear Momentum: $\operatorname{div}(v) = 0$

$$\rho \dot{v} - \operatorname{div} \left(-pI + 2\mu_s D(v) + T_e \right) = \rho f$$

Conformation Tensor: $B = (We/\mu_p)T_e + I$ is SPD

$$\dot{B} - (\nabla v)B - B(\nabla v)^T + (1/We)B = (1/We)I$$

Classical Energy Estimate:

- ▶ Multiply the linear momentum equation by v
- ▶ Take the trace of the equation for B
- ▶ Take the dot product of the equation for B with B^{-1}

Problem (HWNP): If $B_h \in \mathbb{B}_h \subset H^1(\Omega)$ (Lagrange elements)

- ▶ Typically B_h will not be positive definite
- ▶ $B_h^{-1} \notin \mathbb{B}_h$ even if it exists

Plasticity Models

Balance of Mass: $\rho_t + \operatorname{div}(\rho v) = 0$

Linear Momentum:

$$\rho \dot{v} - \operatorname{div} \left(\rho W^\top D\mathcal{W}(W) \right) = \rho f$$

Defect Kinematics:

$$\dot{W} + W(\nabla v) + \mathcal{D}(\operatorname{curl}(W), D\mathcal{W}(W)) = 0$$

Model:

- ▶ Defect Density: $\operatorname{curl}(W)$ (classical elasticity $W \simeq \nabla u$)
- ▶ Elastic Deformation: $W \simeq F^{-1}$
- ▶ Piola Stress: $D\mathcal{W}(W)$
- ▶ Dissipation: $\mathcal{D}(\operatorname{curl}(W), D\mathcal{W}(W))$

Plasticity Models

Balance of Mass: $\rho_t + \operatorname{div}(\rho v) = 0$

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$$\rho \dot{v} - \operatorname{div} \left(\rho W^\top D\mathcal{W}(W) \right) = \rho f$$

Defect Kinematics:

$$\dot{W} + W(\nabla v) + \mathcal{D}(\operatorname{curl}(W), D\mathcal{W}(W)) = 0$$

Energy Estimate:

- ▶ Multiply the linear momentum equation by v
- ▶ Multiply the kinematic equation by $D\mathcal{W}(W)$

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} ((\rho/2)|v|^2 + \mathcal{W}(W)) \\ + \int_{\Omega} \rho \mathcal{D}(\operatorname{curl}(W), D\mathcal{W}(W)) : D\mathcal{W}(W) = \int_{\Omega} (\rho f \cdot v) \end{aligned}$$

Plasticity Models

Balance of Mass: $\rho_t + \operatorname{div}(\rho v) = 0$

Linear Momentum:

$$\rho \dot{v} - \operatorname{div} \left(\rho W^\top D\mathcal{W}(W) \right) = \rho f$$

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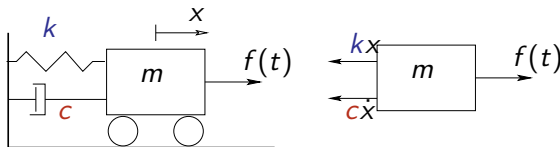
Energy Estimate:

- ▶ Multiply the linear momentum equation by v
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Problems:

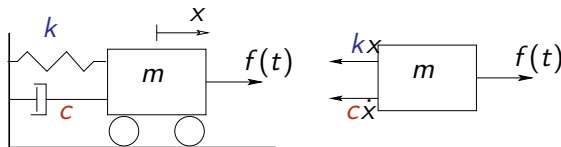
- ▶ If $W_h \in \mathbb{W}_h$ typically $D\mathcal{W}(W_h) \notin \mathbb{W}_h$
- ▶ $\mathcal{D}(\operatorname{curl}(W), D\mathcal{W}(W)) : D\mathcal{W}(W) \not\leq |\operatorname{curl}(W)|^2$

First Order Evolution Equations



Newton's 2nd Law: $m\ddot{x} + c\dot{x} + kx = f$

First Order Evolution Equations



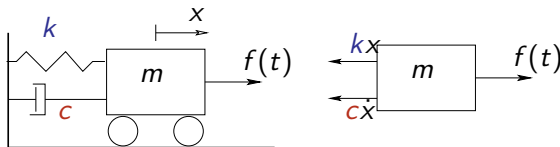
Newton's 2nd Law: $m\ddot{x} + c\dot{x} + kx = f$

1. Negligible Elasticity: $k = 0$ so $m\dot{v} + cv = f$

$$(m/2)v^2(t) + \int_0^t c v^2 = (m/2)v^2(0) + \int_0^t f v$$

Parabolic Equations: Navier Stokes' equations

First Order Evolution Equations



Newton's 2nd Law: $m\ddot{x} + c\dot{x} + kx = f$

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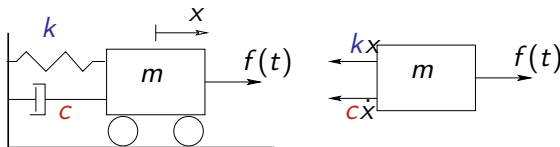
$$(m/2)v^2(t) + \int_0^t c v^2 = (m/2)v^2(0) + \int_0^t f v$$

Parabolic Equations: Navier Stokes' equations

2. Negligible Inertia: $m = 0$ so $c\dot{x} + kx = f$

$$c\dot{x} = -K'(x) \quad \text{where} \quad K(x) = (k/2)x^2 - fx$$

First Order Evolution Equations



Newton's 2nd Law: $m\ddot{x} + c\dot{x} + kx = f$

1. Negligible Elasticity: $k = 0$ so $m\dot{v} + cv = f$

$$(m/2)v^2(t) + \int_0^t c v^2 = (m/2)v^2(0) + \int_0^t f v$$

Parabolic Equations: Navier Stokes' equations

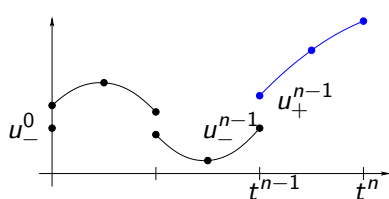
2. Negligible Inertia: $m = 0$ so $c\dot{x} + kx = f$

$$(k/2)x^2(t) + \int_0^t c \dot{x}^2 = (k/2)x^2(0) + \int_0^t f \dot{x}$$

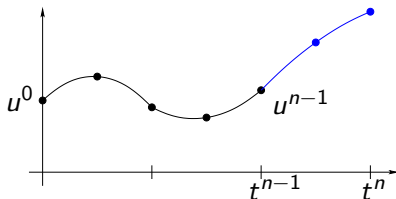
Gradient Flows: Microbiology, Plasticity, Viscoelasticity

Time Stepping Schemes

Time Partition: $0 = t^0 < t^1 < \dots < t^N = T$



DG Time Stepping Scheme



CG Time Stepping Scheme

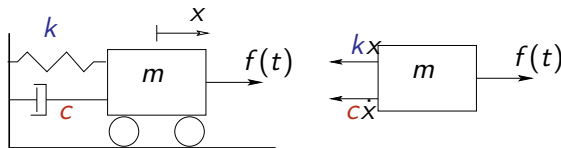
$$\frac{du}{dt} + Au = f, \quad u(0) = u^0$$

“Rule of Thumb”

- ▶ Monotone Operators: $\langle A(u), u \rangle \geq 0$ use DG
- ▶ Gradient Flows: $A(u) = D\mathcal{W}(u)$ use CG

Momentum Equation

Hamilton's Principle



Newton's 2nd Law: $m\ddot{x} + c\dot{x} + kx = f$

Hamilton's Principle: $x(t) \mapsto x(t) + \delta x(t)$

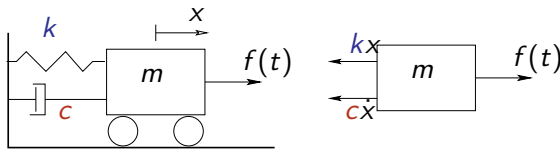
$$\delta \int_{t_1}^{t_2} (\text{Kinetic} - \text{Potential}) \text{ Energy} = \int_{t_1}^{t_2} (\text{Work done by forces})$$

$$\delta \int_{t_1}^{t_2} (1/2)(m\dot{x}^2 - kx^2) = \int_{t_1}^{t_2} (-f + c\dot{x})\delta x$$

$$\int_{t_1}^{t_2} (m\dot{x}\delta\dot{x} - kx\delta x) = \int_{t_1}^{t_2} (-f + c\dot{x})\delta x$$

Momentum Equation

Hamilton's Principle



Newton's 2nd Law: $m\ddot{x} + c\dot{x} + kx = f$

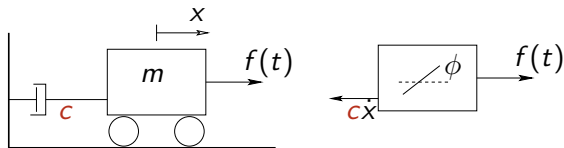
Hamilton's Principle: $x(t) \mapsto x(t) + \delta x(t)$

$$\delta \int_{t_1}^{t_2} (\text{Kinetic} - \text{Potential}) \text{ Energy} = \int_{t_1}^{t_2} (\text{Work done by forces})$$

Energy Estimate: Set $\delta x = \dot{x}$

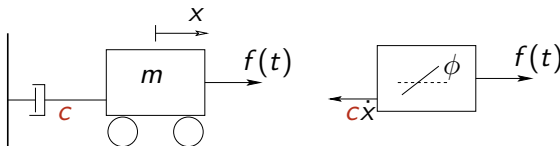
$$E(t) + \int_0^t c \dot{x}^2 = E(0) + \int_0^t f \dot{x} \quad \text{where} \quad E \equiv \frac{1}{2}(m\dot{x}^2 + kx^2)$$

Internal Variables



Question: If $x \mapsto x + \delta x$ what is $\delta \phi$?

Internal Variables



Case 1: δx and $\delta \phi$ are independent (liquid crystals)

- Elastic Coupling: $\mathcal{W}(\phi - \Phi(x))$
- Viscous Coupling: $\mathcal{R}(v, \dot{\phi})$

$$\delta \int_{t_1}^{t_2} (m/2)(\dot{x}^2 + \dot{\phi}^2) - \mathcal{W}(\phi - \Phi(x)) = \int_{t_1}^{t_2} (-f + \frac{\partial \mathcal{R}}{\partial \dot{x}}) \delta x + (-g + \frac{\partial \mathcal{R}}{\partial \dot{\phi}}) \delta \phi$$

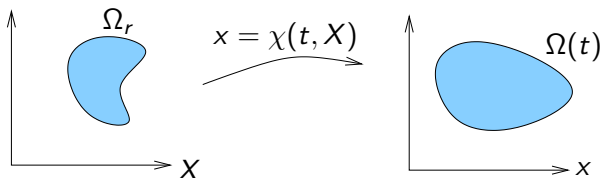
Momentum Equations:

$$m\dot{v} + \frac{\partial \mathcal{R}}{\partial v} - \mathcal{W}'(\phi - \Phi)\Phi' = f$$

$$\frac{\partial \mathcal{R}}{\partial \dot{\phi}} + \mathcal{W}'(\phi - \Phi) = g$$

Hamilton's Principle

$$\delta \int_{t_1}^{t_2} (\text{Kinetic} - \text{Potential}) \text{ Energy} = \int_{t_1}^{t_2} \text{work done}$$



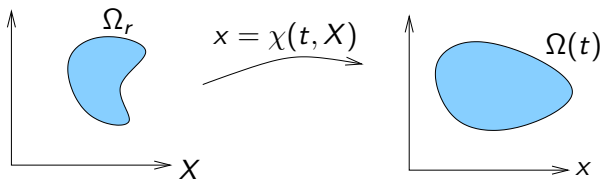
Classical Continuum Mechanics: $x(t, X) \mapsto x(t, X) + \delta x(t, X)$

$$\begin{aligned} \delta \int_{t_1}^{t_2} \int_{\Omega_r} \left((1/2) |\dot{x}(t, X)|^2 - \mathcal{W} \right) \rho_r(X) dX dt \\ = \int_{t_1}^{t_2} \int_{\Omega(t)} \left(-f(t, x) \cdot \delta x + T_v : (\nabla_x \delta x) \right) \rho(t, x) dx dt \end{aligned}$$

Density: $\rho(t, x) dx = \rho_r(X) dX$

Hamilton's Principle

$$\delta \int_{t_1}^{t_2} (\text{Kinetic} - \text{Potential}) \text{ Energy} = \int_{t_1}^{t_2} \text{work done}$$



Nematic Fluids $(x, n) \mapsto (x + \delta x, n + \delta n)$ with $\delta n \cdot n = 0$

$$\begin{aligned} & \delta \int_{t_1}^{t_2} \int_{\Omega_r} \{ (\rho_r/2) (|\dot{x}|^2 + \bar{r}^2 |\dot{n}|^2) dX - \mathcal{W} \} dt \\ &= \int_{t_1}^{t_2} \int_{\Omega(t)} -\rho(f \cdot \delta x + g \cdot \delta n) + T_v : (\nabla \delta x + W(\delta n)) + C_v : (\nabla \delta n) \end{aligned}$$

Axial Vector: $W(\delta n)n = \delta n \times n \in TS_n^2$

Constitutive Relations

Elastic Stresses: Oseen Frank strain energy $\mathcal{W}(n, \nabla n)$

Elastic Cauchy Stress: $x \mapsto x + \delta x$

$$\begin{aligned}\delta_x \int_{t_1}^{t_2} \int_{\Omega(t)} \mathcal{W}(n, \nabla n) &= \int_{t_1}^{t_2} \int_{\Omega(t)} \mathcal{W} \operatorname{div}(\delta x) - (\nabla n)^T \left[\frac{\partial \mathcal{W}}{\partial \nabla n} \right] : (\nabla \delta x) \\ &\equiv \int_{t_1}^{t_2} \int_{\Omega(t)} T_e : (\nabla \delta x)\end{aligned}$$

Elastic Couple Stress: $n \mapsto n + \delta n$

$$\begin{aligned}\delta_n \int_{t_1}^{t_2} \int_{\Omega(t)} \mathcal{W}(n, \nabla n) &= \int_{t_1}^{t_2} \int_{\Omega(t)} \left(\frac{\partial \mathcal{W}}{\partial n} \right) \cdot \delta n + \left[\frac{\partial \mathcal{W}}{\partial \nabla n} \right] : (\nabla \delta n) \\ &\equiv \int_{t_1}^{t_2} \int_{\Omega(t)} g_e \cdot \delta n + C_e : (\nabla \delta n)\end{aligned}$$

Identity: (Lin-Liu) $(\delta \mathcal{W} / \delta x) = (\nabla n)^T (\delta \mathcal{W} / \delta n)$

Constitutive Relations

Transport (Lie Derivative): $\dot{n} = \dot{n} - W(v)n$

Dissipation (Leslie): Most general frame indifferent expression linear in the gradients ... six coefficients

$$\begin{aligned} T_v &= \hat{\gamma}_2(D(v)n \otimes n)_{sym} + \hat{\gamma}_1(\dot{n} \otimes n)_{sym} + \gamma_0(n^T D(v)n)n \otimes n \\ &\quad - \gamma_2(D(v)n \otimes n)_{skew} - \gamma_1(\dot{n} \otimes n)_{skew} + \mu D(v) \end{aligned}$$

$$g_v = \gamma_2 D(v)n + \gamma_1 \dot{n}$$

Restriction:

$$\begin{aligned} \int_{\Omega} (T_v, \nabla v) + (g_v, \dot{n}) &= \gamma_0(n^T D(v)n)^2 + \gamma_1|\dot{n}|^2 + \hat{\gamma}_2|D(v)n|^2 \\ &\quad + (\hat{\gamma}_1 + \gamma_2)\dot{n}^T D(v)n \\ &\geq c_v \left((n^T D(v)n)^2 + |\dot{n}|^2 + |D(v)n|^2 \right) \end{aligned}$$

Constitutive Relations

Transport (Lie Derivative): $\dot{n} = \dot{n} - W(v)n$

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$$\begin{aligned} T_v &= \hat{\gamma}_2(D(v)n \otimes n)_{sym} + \hat{\gamma}_1(\dot{n} \otimes n)_{sym} + \gamma_0(n^T D(v)n)n \otimes n \\ &\quad - \gamma_2(D(v)n \otimes n)_{skew} - \gamma_1(\dot{n} \otimes n)_{skew} + \mu D(v) \end{aligned}$$

$$g_v = \gamma_2 D(v)n + \gamma_1 \dot{n}$$

Parodi Condition: If $\hat{\gamma}_1 = \gamma_2$ then

$$T_v = \left[\frac{\partial \mathcal{R}}{\partial \nabla v} \right] \quad \text{and} \quad g_v = \left(\frac{\partial \mathcal{R}}{\partial \dot{n}} \right)$$

where

$$\mathcal{R} \equiv (\gamma_0/2)(n^T D(v)n)^2 + (\hat{\gamma}_2/2)|n \otimes D(v)n|^2 + (\gamma_1/2)|\dot{n}|^2 + \gamma_2 \dot{n}^T D(v)n$$

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Angular Momentum Equation: $|n| = 1$

$$g_v + g_e - \operatorname{div}(C_e) + \lambda n = \rho g$$

Essential Structure:

$$m \dot{v} + \frac{\partial \mathcal{R}}{\partial v} - \mathcal{W}'(\phi - \Phi) \Phi' = f$$
$$\frac{\partial \mathcal{R}}{\partial \dot{\phi}} + \mathcal{W}'(\phi - \Phi) = g$$

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Essential Structure:

$$\begin{aligned} m\dot{v} + \frac{\partial \mathcal{R}}{\partial v} - \mathcal{W}'(\phi - \Phi)\Phi' &= f \\ \frac{\partial \mathcal{R}}{\partial \dot{\phi}} + \mathcal{W}'(\phi - \Phi) &= g \end{aligned}$$

Alternative Formulation: Eliminate $\mathcal{W}'(\cdot)$ from the first equation

$$m\dot{v} + \frac{\partial \mathcal{R}}{\partial v} + \left(\frac{\partial \mathcal{R}}{\partial \dot{\phi}} - g \right) \Phi' = f$$

Ericksen Leslie Equations

Linear Momentum Equation: $\operatorname{div}(v) = 0$

$$\rho \dot{v} - \operatorname{div}(-pl + \mu D(v) + T_v + T_e) = \rho f$$

Angular Momentum Equation: $|n| = 1$

$$g_v + g_e - \operatorname{div}(C_e) + \lambda n = \rho g$$

Reformulation:

$$\begin{aligned}\operatorname{div}(T_e) &= (\nabla n)^\top (g_e - \operatorname{div}(C_e)) \\ &= (\nabla n)^\top (\rho g - g_v - \lambda n)\end{aligned}$$

Linear Momentum Equation:

$$\rho \dot{v} - \operatorname{div}(-pl + \mu D(v) + T_v) + (\nabla n)^\top g_v = \rho(f + (\nabla n)^\top g)$$

Weak Formulation (njw)

Linear Momentum: $\operatorname{div}(v) = 0$

$$\begin{aligned} \int_{\Omega} (\rho \dot{v}, w) - (p, \operatorname{div}(w)) + (\mu D(v), D(w)) \\ + (T_v, \nabla w) + (g_v, (w \cdot \nabla)n) = \int_{\Omega} (\rho f, w) + (\rho g, (w \cdot \nabla)n) \end{aligned}$$

Angular Momentum:

$$\int_{\Omega} (g_v, m) + \left(\left(\frac{\partial \mathcal{W}}{\partial n} \right), m \right) + \left(\left[\frac{\partial \mathcal{W}}{\partial \nabla n} \right], \nabla m \right) = \int_{\Omega} (\rho g, m)$$

Energy Estimate:

- ▶ Set $w = v$ in the linear momentum equation
- ▶ Set $m = n_t$ in the angular momentum equation

Weak Formulation (njw)

Linear Momentum: $\operatorname{div}(v) = 0$

$$\begin{aligned} \int_{\Omega} (\rho \dot{v}, w) - (p, \operatorname{div}(w)) + (\mu D(v), D(w)) \\ + (T_v, \nabla w) + (g_v, (w \cdot \nabla)n) = \int_{\Omega} (\rho f, w) + (\rho g, (w \cdot \nabla)n) \end{aligned}$$

Angular Momentum:

$$\int_{\Omega} (g_v, m) + \left(\left(\frac{\partial \mathcal{W}}{\partial n} \right), m \right) + \left(\left[\frac{\partial \mathcal{W}}{\partial \nabla n} \right], \nabla m \right) = \int_{\Omega} (\rho g, m)$$

Energy Estimate: (with suitable boundary conditions)

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} \left\{ (\rho/2) |v|^2 + \mathcal{W} \right\} \\ + \int_{\Omega} \left\{ \mu |D(v)|^2 + (T_v, \nabla v) + (g_v, \dot{n}) \right\} = \int_{\Omega} (\rho f, v) + (\rho g, \dot{n}) \end{aligned}$$

Compactness Properties of the DG Scheme

Discrete Aubin–Lions Theorem

Theorem: (njw) Let $U \hookrightarrow H \hookrightarrow U'$ and $U_h \subset U$.

If

1. $u_h|_{(t_h^{n-1}, t_h^n)} \in \mathcal{P}_\ell[t_h^{n-1}, t_h^n; U_h]$ and

$$\int_{t_h^{n-1}}^{t_h^n} (u_{ht}, v_h)_H + ([u^{n-1}], v_+^{n-1})_H = \int_{t_h^{n-1}}^{t_h^n} \langle F_h, v_h \rangle,$$

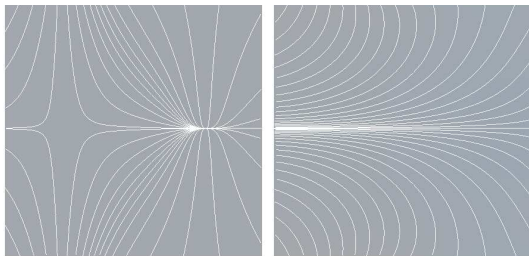
for each $v_h \in \mathcal{P}_\ell[t^{n-1}, t^n; U_h]$.

2. $\{u_h\}_{h>0} \subset L^p[0, T; U]$ is bounded.
3. $\{F_h\}_{h>0} \subset L^q[0, T; U'_h]$ is bounded.

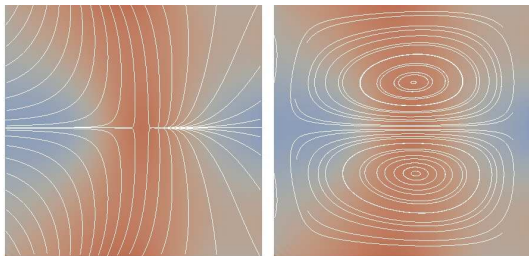
Then $\{u_h\}_{h>0} \subset L^r[0, T; H]$ is compact for $1 \leq r < 2p$.

Annihilation of Singularities

Ericksen Leslie Equations



Director at times
 $t = 0$ and $t = 1$

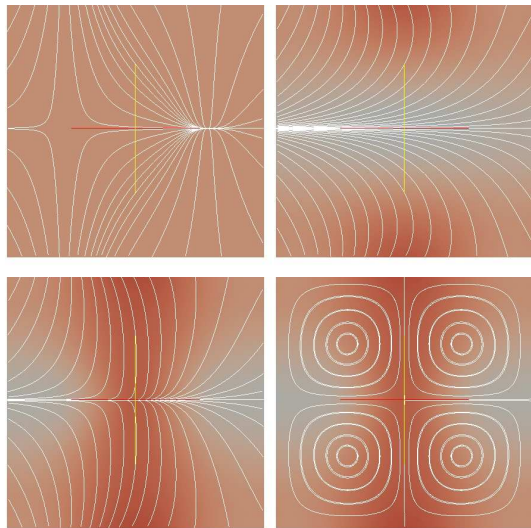


Director and Velocity
at $t = 0.42$
(annihilation)

$$\mathcal{R} = (\gamma_1/2)|\dot{n} - W(v)n|^2 + (\mu/2)|D(v)|^2 \text{ and } \mathcal{W} = (k/2)|\nabla n|^2$$

Annihilation of Singularities

Lin-Liu Equations (gradient flow for n)

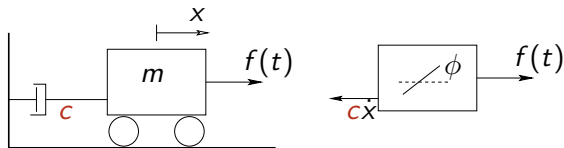


Director at times
 $t = 0$ and $t = 1$

Director and Velocity
at $t = 0.69$
(annihilation)

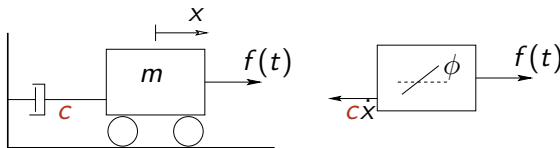
$$\mathcal{R} = (\gamma_1/2)|\dot{n}|^2 + (\mu/2)|D(v)|^2 \text{ and } \mathcal{W} = (k/2)|\nabla n|^2$$

Internal Variables



Question: If $x \mapsto x + \delta x$ what is $\delta \phi$?

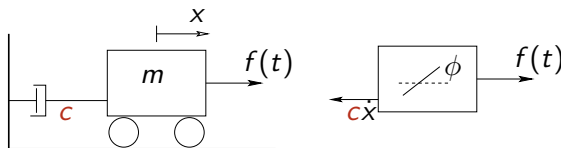
Internal Variables



Case 2: Kinematic coupling $\delta\phi = (\delta x)\phi$ (Oldroyd-B fluid)

- **Kinematics:** Typically $\phi \in G$ a Lie group
- **Macro-Micro:** $\delta x \in \mathcal{G}$ the Lie algebra
cf. Cauchy Born “rule”

Internal Variables



Case 2: Kinematic coupling $\delta\phi = (\delta x)\phi$ (Oldroyd-B fluid)

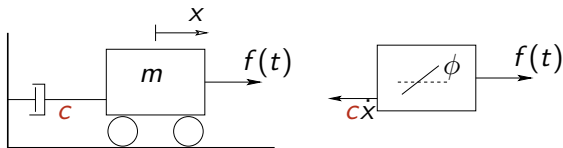
- **Kinematics:** Typically $\phi \in G$ a Lie group
- **Macro-Micro:** $\delta x \in \mathcal{G}$ the Lie algebra

$$\delta \int_{t_1}^{t_2} (m/2) \dot{x}^2 - \mathcal{W}(\phi) = \int_{t_1}^{t_2} (-f + c\dot{x}) \delta x$$

Linear Momentum Equation:

$$m\dot{v} + cv + \mathcal{W}'(\phi)\phi = f$$

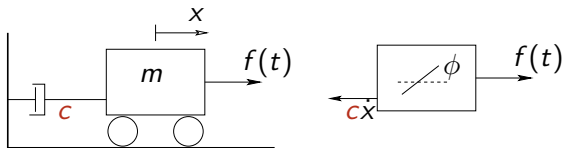
Maximum Dissipation Principle



Instantaneous Response: $\delta\phi - (\delta x)\phi = 0$

Pure Transport: $\dot{\phi} \equiv \dot{\phi} - v\phi = 0$

Maximum Dissipation Principle



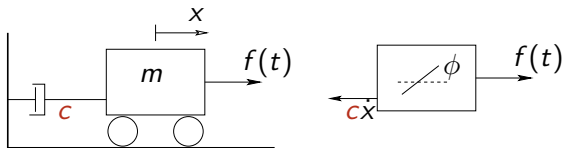
Instantaneous Response: $\delta\phi - (\delta x)\phi = 0$

Pure Transport: $\dot{\phi} \equiv \dot{\phi} - v\phi = 0$

Viscoelasticity: $\mathcal{W}(\phi) \rightsquigarrow 0$

Dissipation: $\mathcal{W}'(\phi)\dot{\phi} \leq 0$

Maximum Dissipation Principle



Instantaneous Response: $\delta\phi - (\delta x)\phi = 0$

Pure Transport: $\dot{\phi} \equiv \dot{\phi} - v\phi = 0$

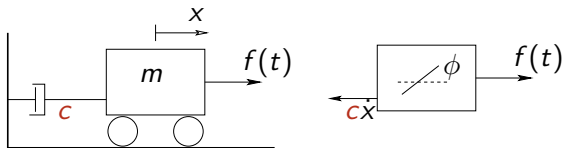
Viscoelasticity: $\mathcal{W}(\phi) \rightsquigarrow 0$

Dissipation: $\mathcal{W}'(\phi) \dot{\phi} \leq 0$

Maximum Dissipation "Principle": $\mu_p \dot{\phi} = -\mathcal{W}'(\phi)$

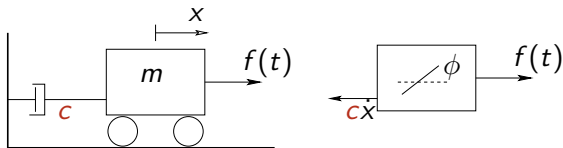
General Dissipation: $\dot{\phi} = -\mathcal{D}(\mathcal{W}'(\phi))$ with $\mathcal{D}$ monotone

Coupled System



$$m\dot{v} + \mu_s v + \mathcal{W}'(\phi)\phi = f$$
$$\dot{\phi} - v\phi + (1/\mu_p)\mathcal{W}'(\phi) = 0$$

Coupled System



$$m\dot{v} + \mu_s v + \mathcal{W}'(\phi)\phi = f$$

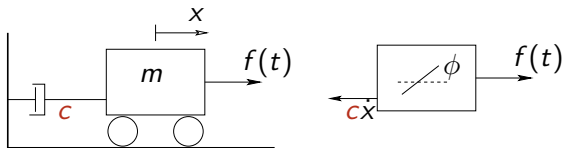
$$\dot{\phi} - v\phi + (1/\mu_p)\mathcal{W}'(\phi) = 0$$

Oldroyd-B Fluid: $T_e \equiv \mathcal{W}'(\phi)\phi$

$$\mathcal{W}'(\phi) = (\mu_p/We)(\phi - 1/\phi) \quad \Rightarrow \quad T_e = (\mu_p/We)(\phi^2 - 1)$$

$$\mathcal{W}(\phi) = (\mu_p/2We) \left(\phi^2 - 1 - \ln(\phi^2) \right)$$

Coupled System



$$m\dot{v} + \mu_s v + \mathcal{W}'(\phi)\phi = f$$

$$\dot{\phi} - v\phi + (1/\mu_p)\mathcal{W}'(\phi) = 0$$

Oldroyd-B Fluid: $T_e \equiv \mathcal{W}'(\phi)\phi$

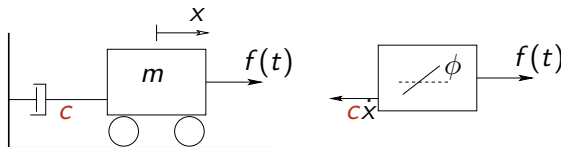
$$\mathcal{W}'(\phi) = (\mu_p/We)(\phi - 1/\phi) \quad \Rightarrow \quad T_e = (\mu_p/We)(\phi^2 - 1)$$

Classical Formulation:

$$m\dot{v} + \mu_s v + T_e = f$$

$$\dot{T}_e - vT_e - T_e v + (2/We)T_e = (2\mu_p/We)v$$

Oldroyd-B Equations



Alternative Formulation:

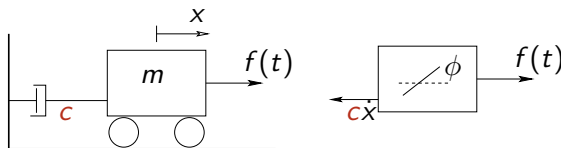
$$m\dot{v} + cv + (\mu_p/We)(\phi^2 - 1) = f$$

$$\dot{\phi} - v\phi + (1/We)(\phi - 1/\phi) = 0$$

Classical Estimate: Multiply by v and $(\mu_p/We)(\phi - 1/\phi)$

$$\frac{d}{dt} \left(\frac{m}{2} v^2 + \frac{\mu_p}{2We} (\phi^2 - 1 - \ln(\phi^2)) \right) + cv^2 + \frac{\mu_p}{We^2} (\phi - 1/\phi)^2 = fv$$

Oldroyd-B Equations



Alternative Formulation:

$$m\dot{v} + cv + (\mu_p/We)(\phi^2 - 1) = f$$
$$\dot{\phi} - v\phi + (1/We)(\phi - 1/\phi) = 0$$

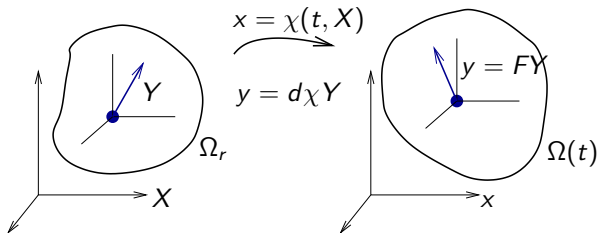
Classical Estimate: Multiply by v and $(\mu_p/We)(\phi - 1/\phi)$

Alternative Estimate: Multiply by v and $(\mu_p/We)\phi$

$$\frac{d}{dt} \left(\frac{m}{2} v^2 + \frac{\mu_p}{2We} \phi^2 \right) + cv^2 + \frac{\mu_p}{We^2} \phi^2 = \left(f + \frac{\mu_p}{We} \right) v + \frac{\mu_p}{We^2}$$

Classical Elasticity

Transport of Tangent Vectors



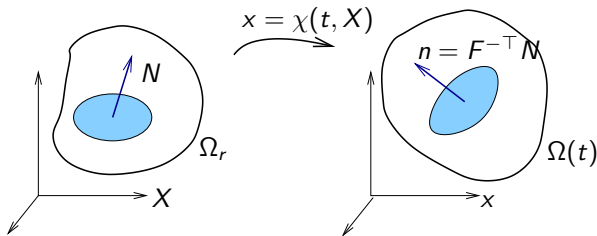
Jacobian: $\delta F = (\nabla \delta x) F$ $F_{i\alpha} \equiv [\partial x_i / \partial X_\alpha]$

Elastic Stress:

$$\delta \mathcal{W}(F) = D\mathcal{W}(F) : (\nabla \delta x) F \quad \Rightarrow \quad T_e = D\mathcal{W}(F) F^\top$$

Classical Fluids

Transport of Normal Vectors (disks & loops)



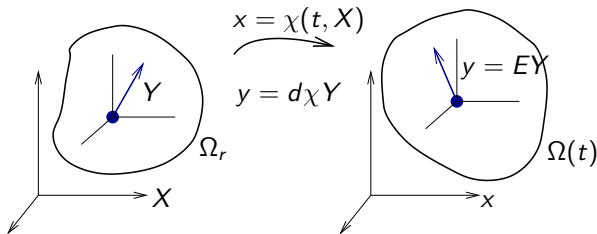
Cofactor: $\delta(F^{-\top}) = -(\nabla_x \delta x)^\top F^{-\top}$

Elastic Stress: $W = F^{-\top}$

$$\delta \mathcal{W}(W) = -D\mathcal{W}(W) : (\nabla \delta x)^\top W \quad \Rightarrow \quad T_e = -W D\mathcal{W}(W)^\top$$

Visco-Elasticity

Oldroyd-B Fluid



Instantaneous Response: $\delta E = (\nabla \delta x) E$

Elastic Stress: $T_e = D\mathcal{W}(E)E^\top$

Oldroyd-B Energy: $\sigma = \mu_p / We$

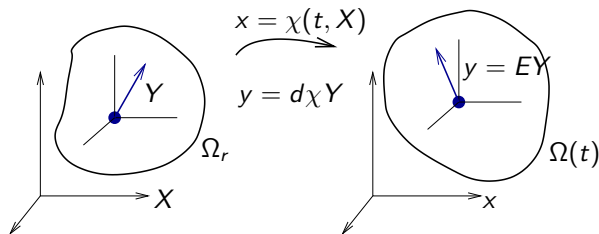
$$\mathcal{W}(E) = (\sigma/2) (|E|^2 - |I|^2 - \ln(\det(E)^2))$$

$$D\mathcal{W}(E) = \sigma (E - E^{-\top})$$

$$T_e = \sigma (EE^\top - I)$$

Visco-Elasticity

Oldroyd-B Fluid



Instantaneous Response: $\delta E = (\nabla \delta x)E$

Elastic Stress: $T_e = D\mathcal{W}(E)E^\top$

Relaxation: $\mathcal{W}(E) \rightarrow 0$

Maximal Dissipation “Principle”: Gradient flow for $\mathcal{W}(\cdot)$

$$\dot{E} - (\nabla v)E = \frac{-1}{2We}(E - E^{-\top})$$

Weak Statement (njw)

Oldroyd-B Fluid

Weak Statement: $\operatorname{div}(v) = 0$

$$\int_{\Omega} (\rho \dot{v}, w) - (p, \operatorname{div}(w)) + 2\mu_s (D(v), D(w)) + \frac{\mu_p}{We} (EE^{\top} - I, (\nabla w)) = \int_{\Omega} (\rho f, w)$$

$$\int_{\Omega} (\dot{E} - (\nabla v)E, G) + \frac{1}{2We} (E - E_{\epsilon}^{-\top}, G) = 0$$

Weak Statement (njw)

Oldroyd-B Fluid

Weak Statement: $\operatorname{div}(v) = 0$

$$\int_{\Omega} (\rho \dot{v}, w) - (p, \operatorname{div}(w)) + 2\mu_s (D(v), D(w)) + \frac{\mu_p}{We} (EE^{\top} - I, (\nabla w)) = \int_{\Omega} (\rho f, w)$$

$$\int_{\Omega} (\dot{E} - (\nabla v)E, G) + \frac{1}{2We} (E - E_{\epsilon}^{-\top}, G) = 0$$

Regularized Inverse: $E_{\epsilon}^{-\top} = \frac{1}{\det_{\epsilon}(E)} \operatorname{Cof}(E)$

$$\det_{\epsilon}(E) = (1/2) \left(\sqrt{\det(E)^2 + 4\epsilon^2 + \epsilon^2 |E|^{2(d-1)}} + \det(E) \right)$$

$x \mapsto 1/x$ is monotone on $(0, \infty)$ with Yosida approximation
 $2/(\sqrt{x^2 + 4\epsilon^2} + x)$

Weak Statement (njw)

Oldroyd-B Fluid

Weak Statement: $\operatorname{div}(v) = 0$

$$\int_{\Omega} (\rho \dot{v}, w) - (p, \operatorname{div}(w)) + 2\mu_s (D(v), D(w)) + \frac{\mu_p}{We} (EE^{\top} - I, (\nabla w)) = \int_{\Omega} (\rho f, w)$$

$$\int_{\Omega} (\dot{E} - (\nabla v)E, G) + \frac{1}{2We} (E - E_{\epsilon}^{-\top}, G) = 0$$

Regularized Inverse: $E_{\epsilon}^{-\top} = \frac{1}{\det_{\epsilon}(E)} \operatorname{Cof}(E)$

Energy Estimate: Set $w = v$ and $G = E$

$$\frac{d}{dt} \int_{\Omega} \frac{\rho}{2} |v|^2 + \frac{\mu_p}{We} |E|^2 + \int_{\Omega} 2\mu_s |D(v)|^2 + \frac{\mu_p}{2We^2} |E|^2 \leq \int_{\Omega} (\rho f \cdot v) + \frac{\mu_p}{2We^2} |I|^2$$

Theorem: (D. Wang, L. Perrotti, njw)

$\Omega \subset \mathbb{R}^d$ bounded Lipschitz domain, $T > 0$.

- ▶ $We, \mu_s, \mu_p > 0$.
- ▶ (v, E) smooth with $v|_{\partial\Omega} = 0$.
- ▶ $(v_h, p_h, E_h) \in \mathcal{P}_1^{disc}[t^{n-1}, t^n; Q'_2 \times Q_1 \times Q_2^{disc}]$
- ▶ Meshes are quasi-uniform and $c\tau \leq h \leq C\tau$.
- ▶ $c\tau \leq \epsilon \leq C\tau$.

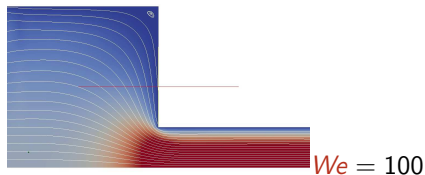
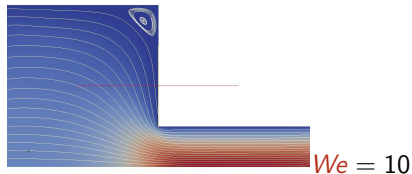
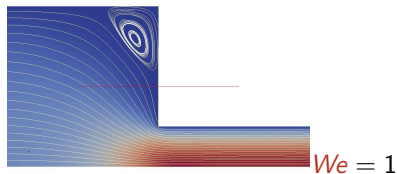
Then there exists constants $C > 0$ and τ_0 independent of (h, τ, ϵ) such that

$$\begin{aligned} & \|v(t_h^n) - v_{h-}^n\|_{L^2(\Omega)}^2 + \|E(t_h^n) - E_{h-}^n\|_{L^2(\Omega)}^2 + \sum_{m=0}^{n-1} \left(\| [v_h^m] \|_{L^2(\Omega)}^2 + \| [E_h^m] \|_{L^2(\Omega)}^2 \right) \\ & + \int_0^{t_h^n} \left(\|D(v - v_h)\|_{L^2(\Omega)}^2 + \|E - E_h\|_{L^2(\Omega)}^2 \right) \leq C (\tau_h^2 + h^2)^2 \end{aligned}$$

provided $\tau \leq \tau_0$

Planar 4 : 1 Contraction

Oldroyd-B Fluid



Streamlines over velocity magnitude (blue small, brown large)

$$T = 2$$

$$\mu = 0.1$$

$$\mu_p = 0.9$$

$$v(t = 2, 4, 0) = 1.0$$

$$v \cdot n = 0 \text{ on } y = 0$$

Dirichlet data otherwise

Parabolic inlet/outlet for v

$$E|_{x=0} \sim \text{Pouiseuille}$$

128 time steps

Crank Nicolson

$$(v_h, p_h, E_h) \in Q'_2 \times Q_1 \times Q_1$$

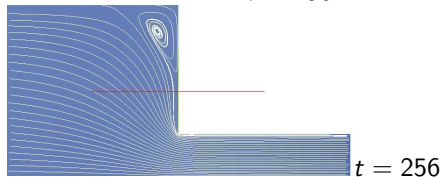
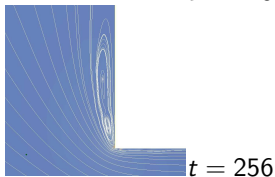
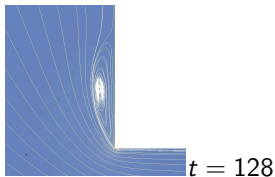
1000 elements

$$10 \times 80 \text{ on } [-4, 0] \times [0, 4]$$

$$10 \times 20 \text{ on } [0, 4] \times [0, 1]$$

Planar 4 : 1 Contraction

Oldroyd-B Fluid



$$\Omega = [-4, 0] \times [0, 4] \cup [0, 4] \times [0, 1]$$

$$\mu_s = 1/9$$

$$\mu_p = 8/9$$

$$We = 2.5$$

$$v(t \geq 1, 4, 0) = 1.5 \text{ (outlet)}$$

$$v \cdot n = 0 \text{ on } y = 0$$

Dirichlet data otherwise

Parabolic inlet/outlet for v

$$E|_{x=0} \sim \text{Pouiseuille}$$

512 time steps

Crank Nicolson

$$(v_h, p_h, E_h) \in Q_1^b \times Q_1 \times Q_1$$

4200 elements

Thank You