Flow and Orientation of Nematic Liquid Crystals

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Overview

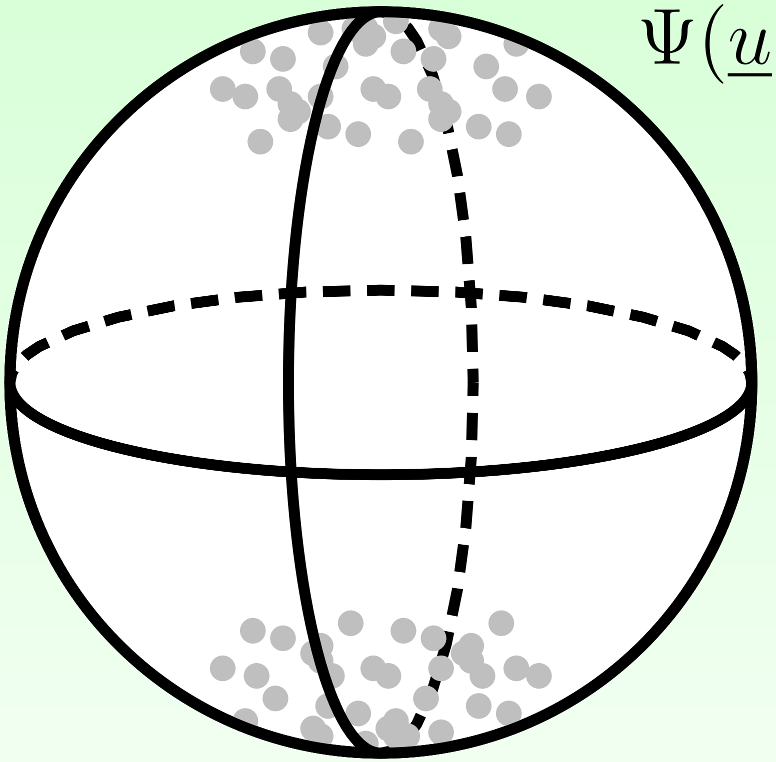
1. Introduction

2. Equations for Flow and Orientation

3. Numerical Method

3. Proof of Concept: Lid Driven Cavity

Nematic Order Parameters



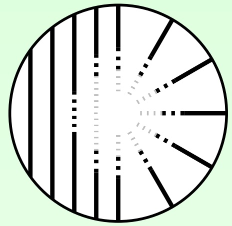
- $\langle f \rangle = \oint_{S^2} f \varrho(\boldsymbol{u}) d^2\boldsymbol{u}$
- $\varrho(\boldsymbol{u}) = \varrho(-\boldsymbol{u})$
- $\varrho(\boldsymbol{u}) = \frac{1}{4\pi}\left(1 + \sum Q_{\mu_1 \ldots \mu_l} \phi_{\mu_1 \ldots \mu_l}\right)$
  with
  $Q_{\mu_1 \ldots \mu_l} = \langle \phi_{\mu_1 \ldots \mu_l} \rangle \propto \langle \overline{u_{\mu_1} \cdots u_{\mu_l}} \rangle$
- $\mathbf{Q} = \sqrt{\frac{3}{2}} \langle \boldsymbol{u} \otimes \boldsymbol{u} - \frac{1}{3}\delta \rangle$
- $\epsilon = \epsilon^{iso}\,\delta + \Delta\epsilon\,\mathbf{Q}$

Alignment Tensor and Relatives

5 $$\mathbf{Q} = S\sqrt{3/2}\,\overline{\boldsymbol{n}\otimes\boldsymbol{n}} + T\sqrt{1/2}\,(\boldsymbol{l}\otimes\boldsymbol{l} - \boldsymbol{m}\otimes\boldsymbol{m})$$

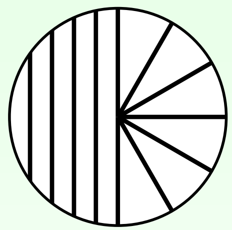
$T = 0$

3 $$\mathbf{Q} = S\sqrt{3/2}\,\overline{\boldsymbol{n}\otimes\boldsymbol{n}}$$



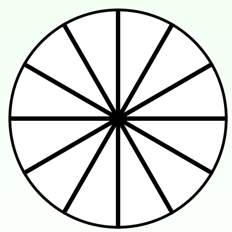
$S = const.$

2 $$\mathbf{Q} = \sqrt{3/2}\,\overline{\boldsymbol{n}\otimes\boldsymbol{n}}$$



Simplified Calculations

2 unit vector $\boldsymbol{n}$



Linear Irreversible Thermodynamics

A recipe for . . .

- Find the *entropy production* in terms of your main players

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Linear Irreversible Thermodynamics

A recipe for . . .

- Find the *entropy production* in terms of your main players
- Write the entropy production as a product of generalised *fluxes and forces*
- Assume that the fluxes are *linear* functions of the forces
- If required, assume that these linear relationships are *symmetric* (Onsager relations)

A brief history . . .

$$\tau_a\left(\frac{\mathrm{d}\mathbf{Q}}{\mathrm{d}t} - 2\,\overline{\mathbf{WQ}} \qquad\qquad\qquad\qquad\right) = \qquad\qquad - \mathbf{\Phi} - \tau_{ap}\sqrt{2}\,\mathbf{D}$$

- S. Hess, *Z. Naturforsch.* 30a (1975)

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$$\tau_a\Big(\frac{\mathrm{d}\mathbf{Q}}{\mathrm{d}t} - 2\,\overline{\mathbf{W}\mathbf{Q}} \qquad\qquad\qquad \Big) = \xi^2\Delta\mathbf{Q} - \mathbf{\Phi} - \tau_{ap}\sqrt{2}\,\mathbf{D}$$

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$$\tau_a\left(\frac{\mathrm{d}\mathbf{Q}}{\mathrm{d}t} - 2\,\overline{\mathbf{W}\mathbf{Q}} - 2\sigma\,\overline{\mathbf{D}\mathbf{Q}}\right) = \xi^2\Delta\mathbf{Q} - \mathbf{\Phi} - \tau_{ap}\sqrt{2}\,\mathbf{D}$$

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- P. D. Olmsted and P. Goldbart, *Phys. Rev. A* 41 (1990) and T. Qian and P. Sheng, *Phys. Rev. E* 58 (1998)

Lagrange Equations with Frictional Forces

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} + \frac{\partial R}{\partial \dot{q}} = 0$$

$$L = T(q, \dot{q}) - V(q)$$
$$q,\, \dot{q} \in \mathbb{R}^m$$

T quadratic in $\dot{q}$

R quadratic in $\dot{q}$

$$\dot{\mathcal{F}} = \dot{T} + \dot{V} = \left(\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q}\right) \cdot \dot{q}$$

$$\frac{\partial R}{\partial \dot{q}} \cdot \dot{q} = 2R$$

$$\dot{\mathcal{F}} + 2R = 0$$

Balance of Forces

Total mechanical power $\mathcal{W} = X \cdot \dot{q}$

↓

Balance of forces $X + Y = 0$

Constitutive Assumption: $$Y = \frac{\partial R}{\partial \dot{q}}$$

↓

Equations of motion $X + \dfrac{\partial R}{\partial \dot{q}} = 0$

Variational principle

In a given configuration the velocities are such that the dissipation R is at a minimum when both the forces X and the power input W are fixed:

$$\delta\mathcal{R} + \lambda\delta\mathcal{W} = \left(\frac{\partial\mathcal{R}}{\partial\dot{q}} + \lambda X\right)\cdot\delta\dot{q} = 0$$

arbitrary $\delta\dot{q}$

$$\lambda X + \frac{\partial\mathcal{R}}{\partial\dot{q}} = 0$$

$\ldots\cdot\dot{q}$

gives $\lambda\mathcal{W} + 2\mathcal{R} = 0$

$$X + \frac{\partial\mathcal{R}}{\partial\dot{q}} = 0$$

Material Frame Indifference

- Material properties must not depend on the observer: Elastic energy and dissipation have to be invariant under Euclidean transformations $\boldsymbol{x}^* = \boldsymbol{\Omega}(t)\boldsymbol{x} + \boldsymbol{b}(t)$
- It is convenient to build the dissipation function from indifferent tensors only. For a velocity field $\boldsymbol{v}$ and an order tensor $\mathbb{O}$ these are, e.g.,
  - $\mathbf{D} = \frac{1}{2}(\nabla\boldsymbol{v} + (\nabla\boldsymbol{v})^T)$
  - $\mathbb{O}$
  - The *corotational* time derivative $\overset{\circ}{\mathbb{O}}$ or a *codeformational* time derivative $\overset{\diamond}{\mathbb{O}}$ of $\mathbb{O}$

Time derivatives . . .

- Material time derivative: $$\dot{\mathbb{O}} = \frac{\partial}{\partial t}\mathbb{O} + (\nabla\mathbb{O})\boldsymbol{v}$$
- Corotational time derivative (JAUMANN):

$$\boxed{\mathring{O}_I = \dot{O}_I - \sum_{\mathrm{k}=1}^{\mathrm{n}} W_{I_{\mathrm{k}}j} O_{I_{\mathrm{k}}^j}}, \qquad \mathbf{W} = \tfrac{1}{2}(\nabla\boldsymbol{v} - (\nabla\boldsymbol{v})^T),$$

$$I = (I_1, \cdots, I_{\mathrm{n}}),\ I_{\mathrm{k}}^j = (I_1, \cdots, I_{\mathrm{k}-1}, j, I_{\mathrm{k}+1}, \cdots, I_{\mathrm{n}})$$

- Codeformational time derivative (OLDROYD):

$$\hat{O}_I = \mathring{O}_I + \sum_{\mathrm{k}=1}^{\mathrm{n}} a_{\mathrm{k}} D_{I_{\mathrm{k}}j} O_{I_{\mathrm{k}}^j}$$

…of the Alignment Tensor

- Material time derivative $\dot{\mathbf{Q}} = \frac{\partial \mathbf{Q}}{\partial t} + (\nabla \mathbf{Q})\boldsymbol{v}$
- …of the gradient $(\nabla \mathbf{Q})^{\cdot} = \nabla \dot{\mathbf{Q}} - (\nabla \mathbf{Q})\nabla \boldsymbol{v}$
- Frame indifferent time derivatives:
  - Co-rotational: $\overset{\circ}{\mathbf{Q}} = \dot{\mathbf{Q}} - 2\,\overline{\mathbf{WQ}}$
  - Co-deformational: $\overset{\diamond}{\mathbf{Q}} = \dot{\mathbf{Q}} - 2\,\overline{\mathbf{WQ}} - 2\sigma\,\overline{\mathbf{DQ}}$

with $\mathbf{D} = \frac{1}{2}(\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T)$ and $\mathbf{W} = \frac{1}{2}(\nabla \boldsymbol{v} - (\nabla \boldsymbol{v})^T)$

Free Energy

$$\mathcal{F} = \int \left\{ \frac{1}{2}\rho \boldsymbol{v}^2 + \chi(\mathbf{Q}) + W(\mathbf{Q}, \nabla\mathbf{Q}) \right\} \mathrm{d}V$$

- ρ: mass density
- χ: potential energy for external actions on $\mathbf{Q}$
- W: elastic free energy of the alignment
- NOT here:
  - potential energy of the compressibility ($\operatorname{div} \boldsymbol{v} = 0$)
  - body force
  - microinertia

Power Input

$$\begin{aligned}
\dot{\mathcal{F}} &= \int \left\{ \rho \dot{\boldsymbol{v}} \cdot \boldsymbol{v} + \left(\frac{\partial \chi}{\partial \mathbf{Q}} + \frac{\partial W}{\partial \mathbf{Q}} \right) \cdot \dot{\mathbf{Q}} + \frac{\partial W}{\partial \nabla \mathbf{Q}} \cdot (\nabla \mathbf{Q})^{\cdot} \right\} \mathrm{d}V \\
&= \int \left\{ \left[\rho \dot{\boldsymbol{v}} + \operatorname{div} \left(p\mathbf{I} + \nabla \mathbf{Q} \odot \frac{\partial W}{\partial \nabla \mathbf{Q}} \right) \right] \cdot \boldsymbol{v} \right. \\
&+ \left. \left[\frac{\partial \chi}{\partial \mathbf{Q}} + \frac{\partial W}{\partial \mathbf{Q}} - \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{Q}} \right] \cdot \dot{\mathbf{Q}} \right\} \mathrm{d}V + \text{s.t.}
\end{aligned}$$

- $$\left(\nabla \mathbf{Q} \odot \frac{\partial W}{\partial \nabla \mathbf{Q}} \right)_{ij} := Q_{kl,i} \frac{\partial W}{\partial Q_{kl,j}}$$

Fluxes and Forces

$\dot{q}$	X
$\boldsymbol{v}$	$\rho\dot{\boldsymbol{v}} + \operatorname{div}\left(p\,\mathbf{I} + \nabla\mathbf{Q} \odot \dfrac{\partial W}{\partial \nabla \mathbf{Q}}\right)$
$\dot{\mathbf{Q}}$	$\dfrac{\partial \chi}{\partial \mathbf{Q}} + \dfrac{\partial W}{\partial \mathbf{Q}} - \operatorname{div} \dfrac{\partial W}{\partial \nabla \mathbf{Q}}$

Dissipation

$$\mathcal{R} = \int R(\mathbf{Q}, \mathring{\mathbf{Q}}, \mathbf{D}) \mathrm{d}V$$

$$\delta(\nabla \boldsymbol{v}) = \nabla(\delta \boldsymbol{v})$$

$$\delta\mathcal{R} = \int \left\{ \frac{\partial R}{\partial \dot{\mathbf{Q}}} \cdot \delta\dot{\mathbf{Q}} + \frac{\partial R}{\partial \nabla \boldsymbol{v}} \cdot \nabla(\delta \boldsymbol{v}) \right\} \mathrm{d}V$$

integration by parts

$$\delta\mathcal{R} = \int \left\{ \frac{\partial R}{\partial \dot{\mathbf{Q}}} \cdot \delta\dot{\mathbf{Q}} - \mathrm{div}\left(\frac{\partial R}{\partial \nabla \boldsymbol{v}} \right) \cdot \delta \boldsymbol{v} \right\} \mathrm{d}V + \mathrm{s.t.}$$

Chain Rule

$$\frac{\partial R}{\partial \nabla \boldsymbol{v}} = \frac{\partial R}{\partial \mathbf{D}} + \mathbf{Q} \frac{\partial R}{\partial \overset{\circ}{\mathbf{Q}}} - \frac{\partial R}{\partial \overset{\circ}{\mathbf{Q}}} \mathbf{Q}$$

$$\frac{\partial R}{\partial \dot{\mathbf{Q}}} = \frac{\partial R}{\partial \overset{\circ}{\mathbf{Q}}}$$

Equations of Motion

$$\rho \dot{\boldsymbol{v}} = \operatorname{div} \mathbf{T}$$

$$\frac{\partial \chi}{\partial \mathbf{Q}} + \frac{\partial W}{\partial \mathbf{Q}} - \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{Q}} + \frac{\partial R}{\partial \overset{\circ}{\mathbf{Q}}} = \mathbf{0}$$

$$\mathbf{T} = -p\,\mathbf{I} - \nabla \mathbf{Q} \odot \frac{\partial W}{\partial \nabla \mathbf{Q}} + \frac{\partial R}{\partial \mathbf{D}} + \mathbf{Q} \frac{\partial R}{\partial \overset{\circ}{\mathbf{Q}}} - \frac{\partial R}{\partial \overset{\circ}{\mathbf{Q}}} \mathbf{Q}$$

15 Invariants Bilinear in $\mathring{\mathbf{Q}}$ and $\mathbf{D}$

$\mathring{\mathbf{Q}}^2$	$\mathbf{D} \cdot \mathring{\mathbf{Q}}$	$\mathbf{D}^2$
$\mathring{\mathbf{Q}} \cdot (\mathring{\mathbf{Q}}\mathbf{Q})$	$\mathring{\mathbf{Q}} \cdot (\mathbf{D}\mathbf{Q})$	$\mathbf{D} \cdot (\mathbf{D}\mathbf{Q})$
$(\mathring{\mathbf{Q}} \cdot \mathbf{Q})^2$	$(\mathbf{D} \cdot \mathbf{Q})(\mathring{\mathbf{Q}} \cdot \mathbf{Q})$	$(\mathbf{D} \cdot \mathbf{Q})^2$
$(\mathring{\mathbf{Q}}\mathbf{Q}) \cdot (\mathring{\mathbf{Q}}\mathbf{Q})$	$(\mathbf{D}\mathbf{Q}) \cdot (\mathring{\mathbf{Q}}\mathbf{Q})$	$(\mathbf{D}\mathbf{Q}) \cdot (\mathbf{D}\mathbf{Q})$
$\mathbf{Q}^2 \mathring{\mathbf{Q}}^2$	$\mathbf{Q}^2 (\mathbf{D} \cdot \mathring{\mathbf{Q}})$	$\mathbf{Q}^2 \mathbf{D}^2$

The Director: $\mathbf{Q} = S\,\overline{\boldsymbol{n} \otimes \boldsymbol{n}}$

$2S^2\mathring{\boldsymbol{n}}^2$	$2S\mathring{\boldsymbol{n}} \cdot \mathbf{D}\boldsymbol{n}$	$\mathbf{D} \cdot \mathbf{D}$
$\frac{1}{3}S^3\mathring{\boldsymbol{n}}^2$	$\frac{1}{3}S^2\mathring{\boldsymbol{n}} \cdot \mathbf{D}\boldsymbol{n}$	$S(\lVert\mathbf{D}\boldsymbol{n}\rVert^2 - \frac{1}{3}\mathbf{D} \cdot \mathbf{D})$
0	0	$S^2(\boldsymbol{n} \cdot \mathbf{D}\boldsymbol{n})^2$
$\frac{5}{9}S^4\mathring{\boldsymbol{n}}^2$	$\frac{5}{9}S^3\mathring{\boldsymbol{n}} \cdot \mathbf{D}\boldsymbol{n}$	$S^2(\frac{1}{9}\mathbf{D} \cdot \mathbf{D} + \frac{1}{3}\lVert\mathbf{D}\boldsymbol{n}\rVert^2)$
$\frac{4}{3}S^4\mathring{\boldsymbol{n}}^2$	$\frac{4}{3}S^3\mathring{\boldsymbol{n}} \cdot \mathbf{D}\boldsymbol{n}$	$\frac{2}{3}S^2\mathbf{D} \cdot \mathbf{D}$

8 Terms up to Second Order in S

$$
\begin{aligned}
R \;=\; & \frac{1}{2}\zeta_1 \mathring{\mathbf{Q}} \cdot \mathring{\mathbf{Q}} + \zeta_2\, \mathbf{D} \cdot \; \mathring{\mathbf{Q}} + \frac{1}{2}\zeta_3\, \mathbf{D} \cdot \mathbf{D} + \\
& \zeta_{21} \mathring{\mathbf{Q}} \; \cdot (\mathbf{D} \cdot \mathbf{Q}) + \\
& \frac{1}{2}\zeta_{31}\, \mathbf{D} \cdot (\mathbf{D}\mathbf{Q}) + \frac{1}{2}\zeta_{32}\, (\mathbf{D} \cdot \mathbf{Q})^2 + \\
& \frac{1}{2}\zeta_{33}\, (\mathbf{D}\mathbf{Q}) \cdot (\mathbf{D}\mathbf{Q}) + \frac{1}{2}\zeta_{34}\, (\mathbf{Q} \cdot \mathbf{Q})(\mathbf{D} \cdot \mathbf{D})
\end{aligned}
$$

Comparison to ELP theory

$$R = \frac{1}{2}\gamma_1 \mathring{\boldsymbol{n}}^2 + \gamma_2 \mathring{\boldsymbol{n}} \cdot \mathbf{D}\boldsymbol{n} + \frac{1}{2}\gamma_3 (\mathbf{D}\boldsymbol{n})^2 + \frac{1}{2}\alpha_1 (\boldsymbol{n} \cdot \mathbf{D}\boldsymbol{n})^2 + \frac{1}{2}\alpha_4 \mathbf{D} \cdot \mathbf{D}$$

with $\gamma_1 = \alpha_3 - \alpha_2$, $\gamma_2 = \alpha_5 - \alpha_6$, $\gamma_3 = \alpha_5 + \alpha_6$.

$$\begin{aligned}
\gamma_1 &= 2S^2\zeta_1 \\
\gamma_2 &= 2S\zeta_2 + \frac{1}{3}S^2\zeta_{21} \\
\gamma_3 &= S\zeta_{31} + \frac{1}{3}S^2\zeta_{33} \\
\alpha_1 &= S^2\zeta_{32} \\
\alpha_4 &= \zeta_3 - \frac{1}{3}S\zeta_{31} + \frac{1}{9}S^2\zeta_{33} + \frac{2}{3}S^2\zeta_{34}
\end{aligned}$$

Further Simplification

$\zeta_{21} = \zeta_{33} = \zeta_{34} = 0$: neglect *corrections* of order S^2:

$$R = \frac{1}{2}\zeta_1 \mathring{\mathbf{Q}}\cdot\mathring{\mathbf{Q}} + \zeta_2 \mathbf{D}\cdot\mathring{\mathbf{Q}} + \frac{1}{2}\zeta_3 \mathbf{D}\cdot\mathbf{D} + \frac{1}{2}\zeta_{31}\mathbf{D}\cdot(\mathbf{D}\mathbf{Q}) + \frac{1}{2}\zeta_{32}(\mathbf{D}\cdot\mathbf{Q})^2.$$

$$W = \phi + \frac{1}{2}L_1\|\nabla\mathbf{Q}\|^2,$$

where $\phi = \frac{1}{2}A(T)\,\mathrm{tr}\,\mathbf{Q}^2 - \frac{\sqrt{6}}{3}B\,\mathrm{tr}\,\mathbf{Q}^3 + \frac{1}{4}C(\mathrm{tr}\,\mathbf{Q}^2)^2$ is the Landau-deGennes potential and L_1 is an elastic modulus.

Equations

$$\zeta_1 \overset{\circ}{\mathbf{Q}} = -\mathbf{\Phi} - \zeta_2 \mathbf{D} + L_1 \Delta \mathbf{Q},$$

and the skew-symmetric part of the stress tensor is

$$\mathbf{T}^{\text{skew}} \;=\; \zeta_1(\mathbf{Q}\overset{\circ}{\mathbf{Q}} - \overset{\circ}{\mathbf{Q}}\mathbf{Q}) + \zeta_2(\mathbf{Q}\mathbf{D} - \mathbf{D}\mathbf{Q})$$

The symmetric traceless part of the viscous stress is given by

$$\overline{\mathbf{T}^{(\text{v})}} = \zeta_2 \overset{\circ}{\mathbf{Q}} + \zeta_3 \mathbf{D} + \zeta_{31}\, \overline{\mathbf{D}\mathbf{Q}} + \zeta_{32}(\mathbf{Q}\cdot\mathbf{D})\,\mathbf{Q},$$

and the elastic contribution to the stress, which here is symmetric, reads as

$$\mathbf{T}^{(\text{e})} = -L_1\, \nabla\mathbf{Q} \odot \nabla\mathbf{Q}.$$

Separating the Time Dependencies

On a solution

$$\overset{\circ}{\mathbf{Q}} = \frac{1}{\zeta_1}\left(-\mathbf{\Phi} - \zeta_2\mathbf{D} + L_1\Delta\mathbf{Q}\right)$$

and so

$$\begin{aligned}
\mathbf{T}^{\mathrm{skew}} &= \zeta_1(\mathbf{Q}\overset{\circ}{\mathbf{Q}} - \overset{\circ}{\mathbf{Q}}\mathbf{Q}) + \zeta_2(\mathbf{QD} - \mathbf{DQ}) \\
&= \mathbf{\Phi Q} - \mathbf{Q\Phi} + L_1[\mathbf{Q}(\Delta\mathbf{Q}) - (\Delta\mathbf{Q})\mathbf{Q}] \\
&= L_1[\mathbf{Q}(\Delta\mathbf{Q}) - (\Delta\mathbf{Q})\mathbf{Q}]
\end{aligned}$$

and

$$\overline{\mathbf{T}^{(\mathrm{v})}} = \frac{\zeta_2}{\zeta_1}\left(L_1\Delta\mathbf{Q} - \mathbf{\Phi}\right) + \zeta_4\mathbf{D} + \zeta_{31}\,\overline{\mathbf{DQ}} + \zeta_{32}(\mathbf{Q}\cdot\mathbf{D})\,\mathbf{Q}$$

with $\zeta_4 := \zeta_3 - \frac{\zeta_2^2}{\zeta_1}$.

Viscosities

With ($\approx$ MBBA)

$$\alpha_1 = \alpha_3 = 0$$
$$\alpha_4 = -\alpha_2 = \alpha$$
$$\alpha_5 = -\alpha_6 = \alpha/2$$

$$\Longrightarrow$$

$$\zeta_1 = \alpha/2S^2$$
$$\zeta_2 = \alpha/2S$$
$$\zeta_3 = \alpha$$
$$\zeta_4 = 3\alpha/2$$
$$\zeta_{31} = \zeta_{32} = 0$$

$$\zeta_{31} = \zeta_{32} = 0$$

$$\operatorname{div} \mathbf{T} = \boldsymbol{0} \Rightarrow$$

$$\nabla p - \frac{1}{2}\zeta_4 \Delta \boldsymbol{v} = \boldsymbol{f}$$

$$\boldsymbol{f} = \operatorname{div} \mathbf{F}$$

$$\mathbf{F} = L_1 \Big(\mathbf{Q}(\Delta \mathbf{Q}) - (\Delta \mathbf{Q})\mathbf{Q} + \tfrac{\zeta_2}{\zeta_1} \Delta \mathbf{Q} - \nabla \mathbf{Q} \odot \nabla \mathbf{Q} \Big) - \tfrac{\zeta_2}{\zeta_1} \mathbf{\Phi}$$

Strategy

1. For a given orientation field $\mathbf{Q}$, solve Stokes equation with $\boldsymbol{f}$ as a body force
2. Use the obtained flow field to compute one time step in a discretised version of the orientation equation
3. With the new orientation field, go back to 1.

Dimensionless Quantities

- $\tilde{\mathbf{Q}} = \frac{3C}{2B}\mathbf{Q}$
- $\tau_1 = \frac{9C\zeta_1}{2B^2}$
- $\xi = \sqrt{\frac{9CL_1}{2B^2}}$
- $\mathrm{Tu} = \frac{3C\zeta_2}{2B\zeta 1}$
- $\mathrm{Bf} = \frac{4B\zeta_2}{3C\zeta_4}$
- $\tilde{\boldsymbol{\Phi}} = (\vartheta + 2\,\mathrm{tr}\,\tilde{\mathbf{Q}}^2)\tilde{\mathbf{Q}} + 3\sqrt{6}\ \overline{\tilde{\mathbf{Q}}\tilde{\mathbf{Q}}}$
- $\vartheta = \frac{9C}{2B^2}A(T)$
- $\tilde{p} = \ldots$

Dimensionless Equations

$$\overset{\circ}{\mathbf{Q}} = \Delta\mathbf{Q} - \boldsymbol{\Phi} - \mathrm{Tu}\,\mathbf{D}$$

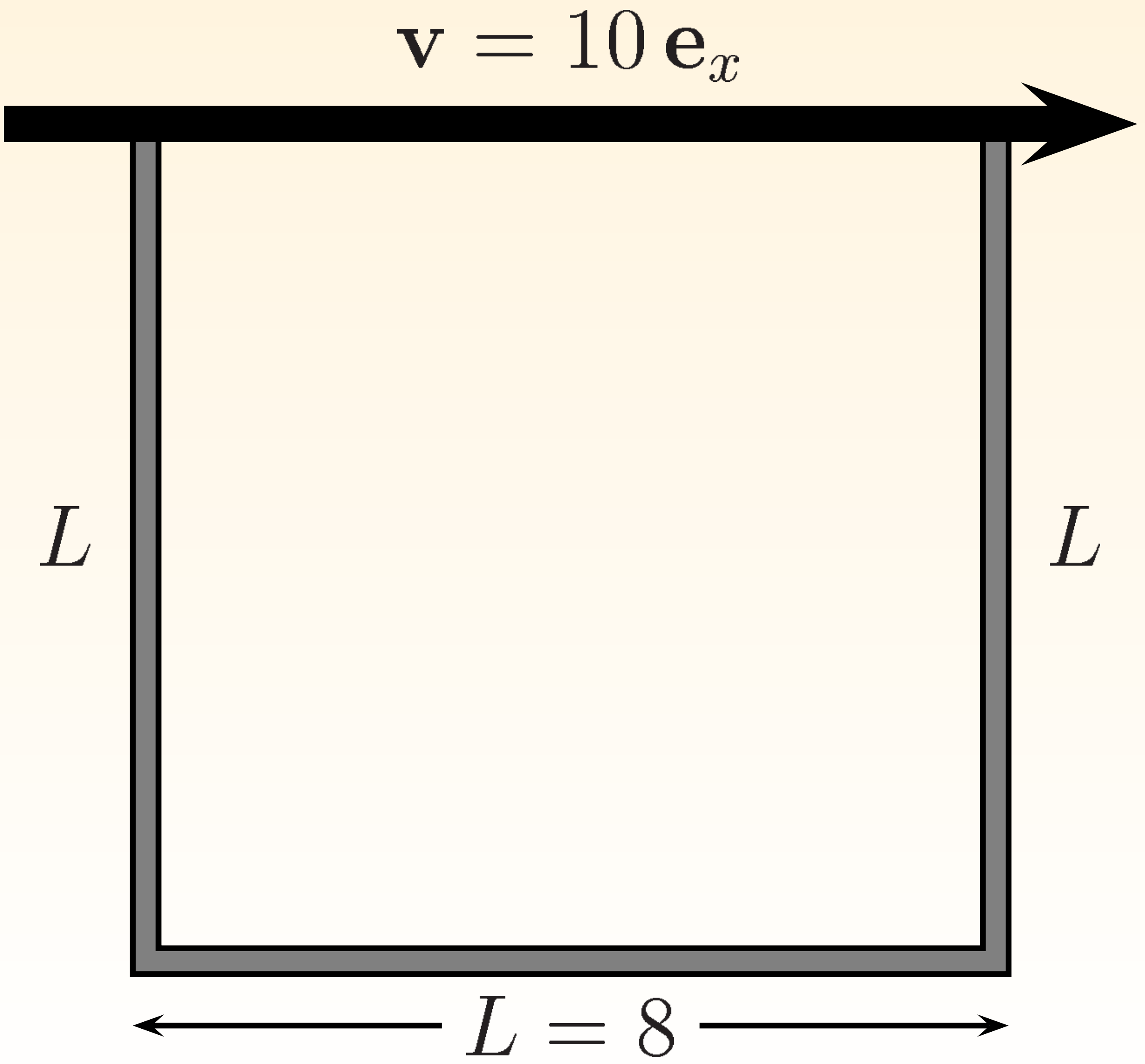
$$\nabla p - \Delta\boldsymbol{v} = \operatorname{div}\mathbf{F}$$

$$\mathbf{F} = \mathrm{Bf}\left\{\frac{1}{\mathrm{Tu}}\left[\mathbf{Q}(\Delta\mathbf{Q}) - (\Delta\mathbf{Q})\mathbf{Q} - \nabla\mathbf{Q}\odot\nabla\mathbf{Q}\right] + \Delta\mathbf{Q} - \boldsymbol{\Phi}\right\}$$

Solving the Equations

- Orientation equation: finite difference scheme with explicit euler time discretisation (leaves a lot of room for improvement . . .)
- Stokes equation: finite element iterative solver. Matlab package using MINRES solver with multigrid preconditioning (this should really be coded using an efficient programming language . . .). http://www.cs.umd.edu/~elman/ifiss.html (Incompressible Flow & Iterative Solver Software Version 2.2)

Lid Driven Cavity



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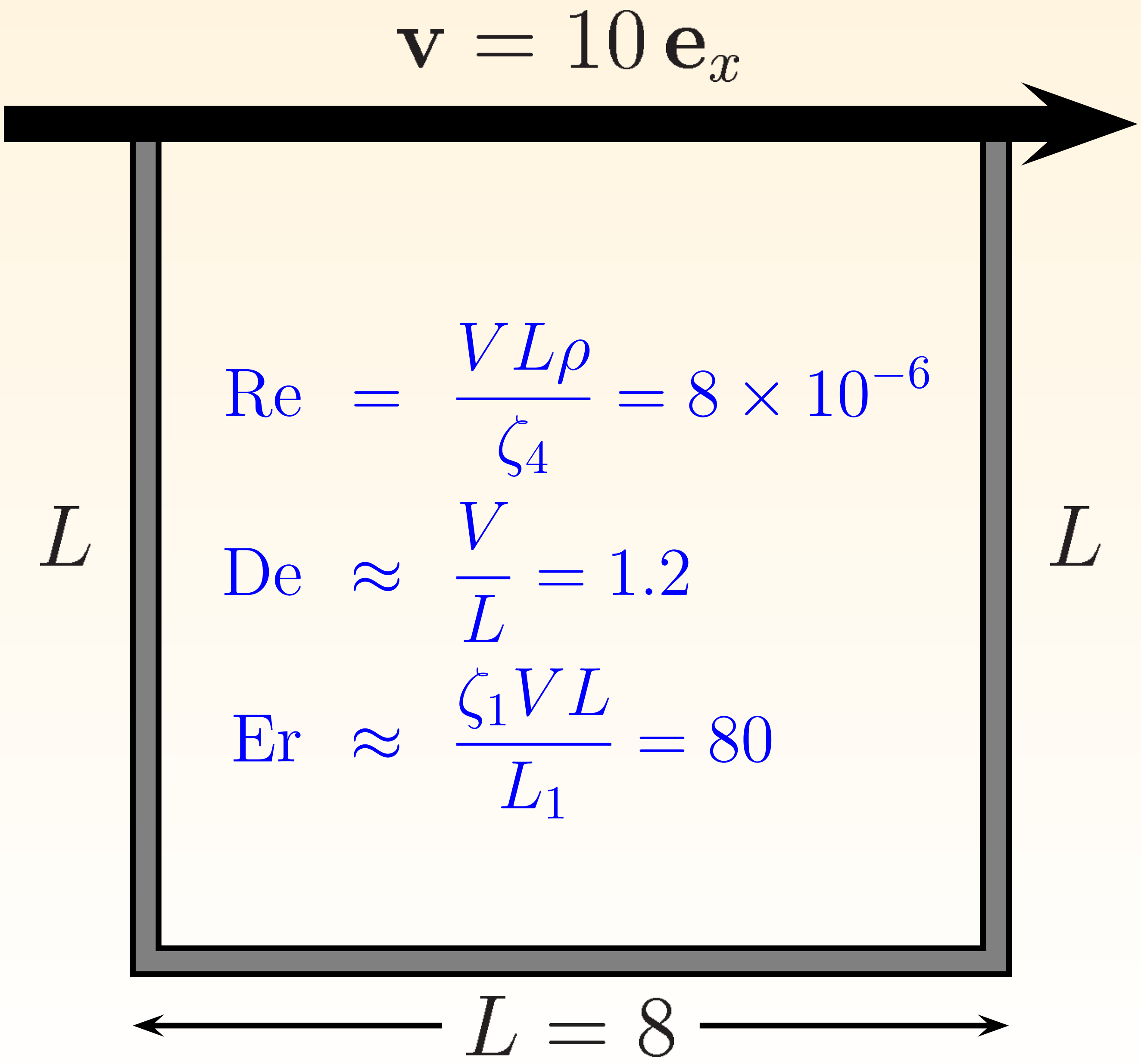


$$\mathrm{Re} = \frac{VL\rho}{\zeta_4} = 8 \times 10^{-6}$$

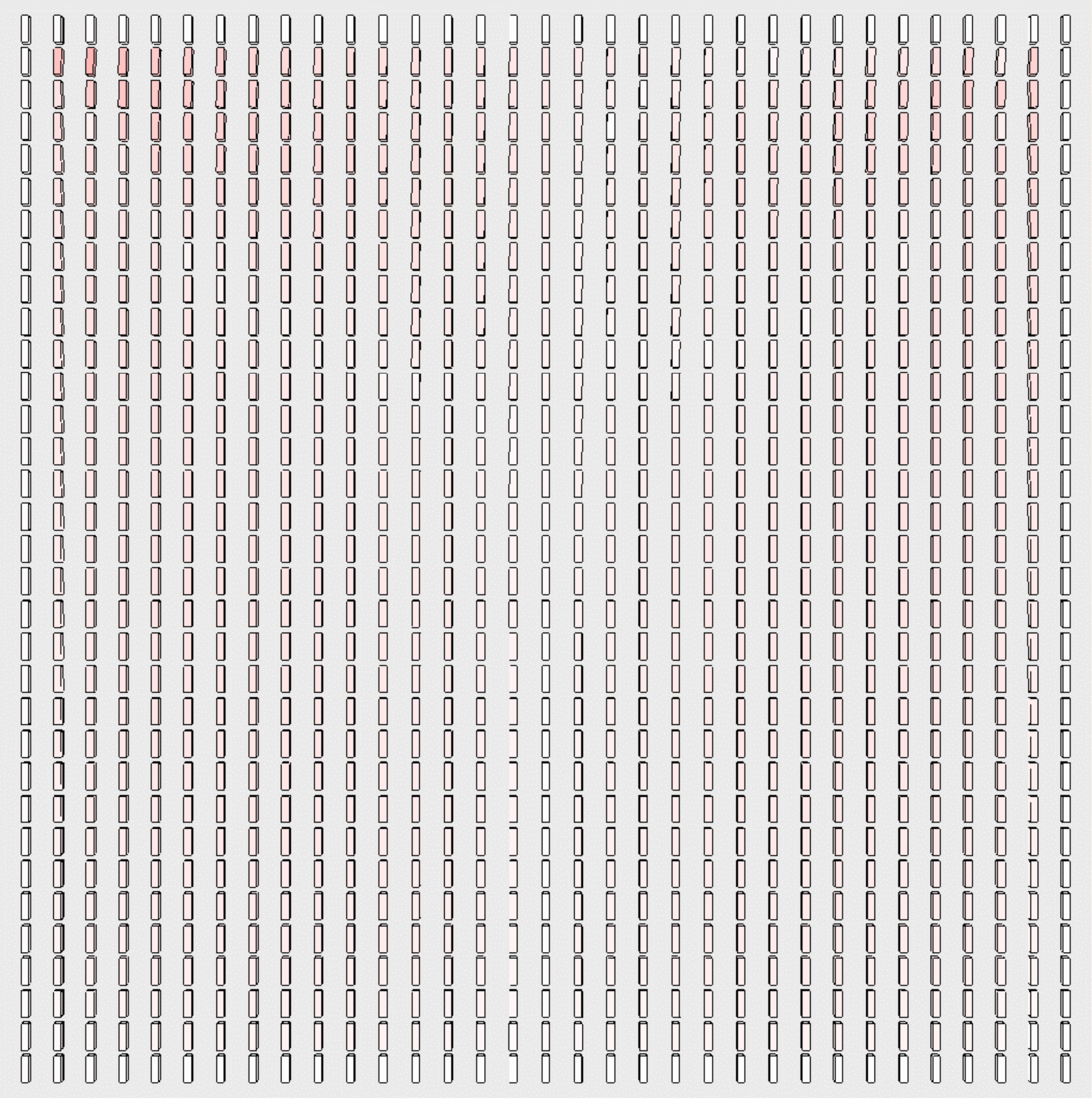
$$\mathrm{De} \approx \frac{V}{L} = 1.2$$

$$\mathrm{Er} \approx \frac{\zeta_1 V L}{L_1} = 80$$

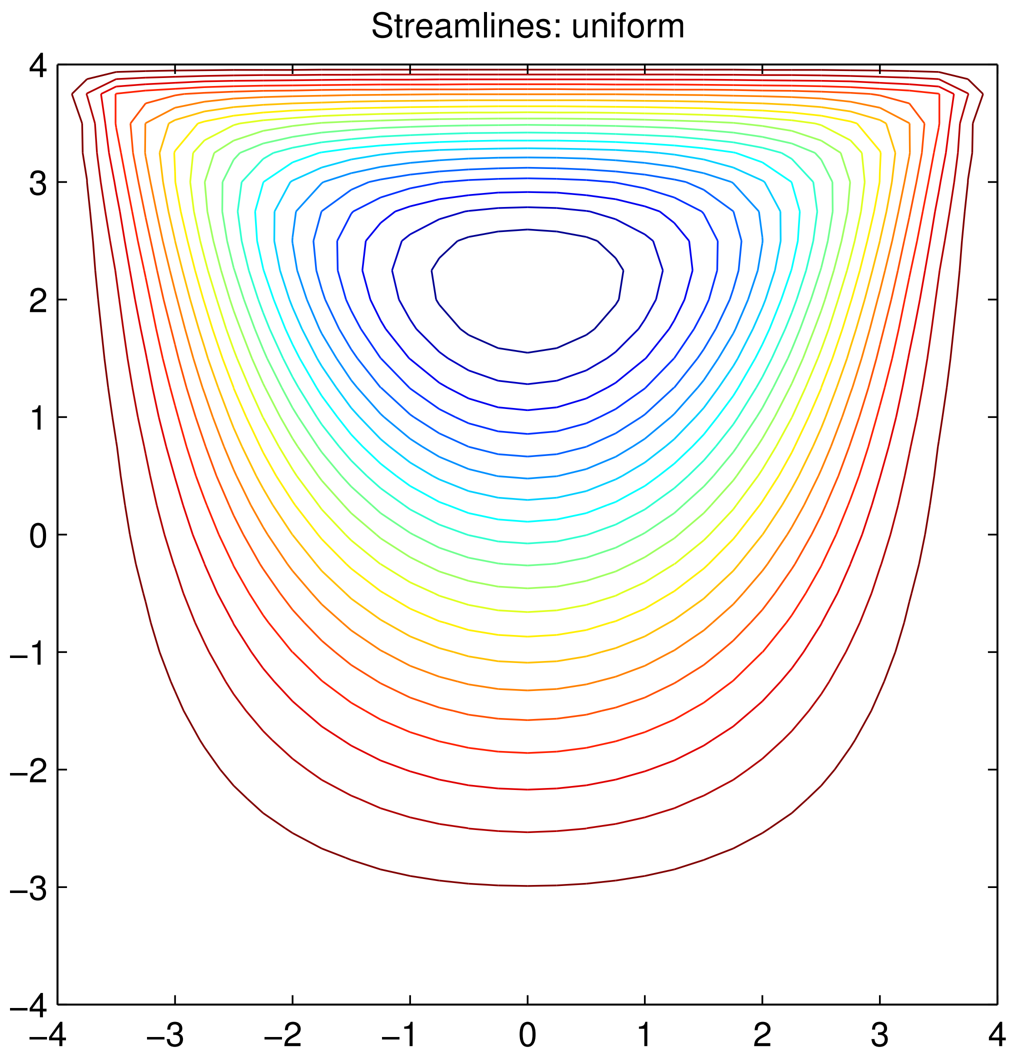
Biaxiality Measure

$$\beta^2 = 1 - \frac{6(\operatorname{tr}\mathbf{Q}^3)^2}{(\operatorname{tr}\mathbf{Q}^2)^3} \qquad \in [0, 1]$$

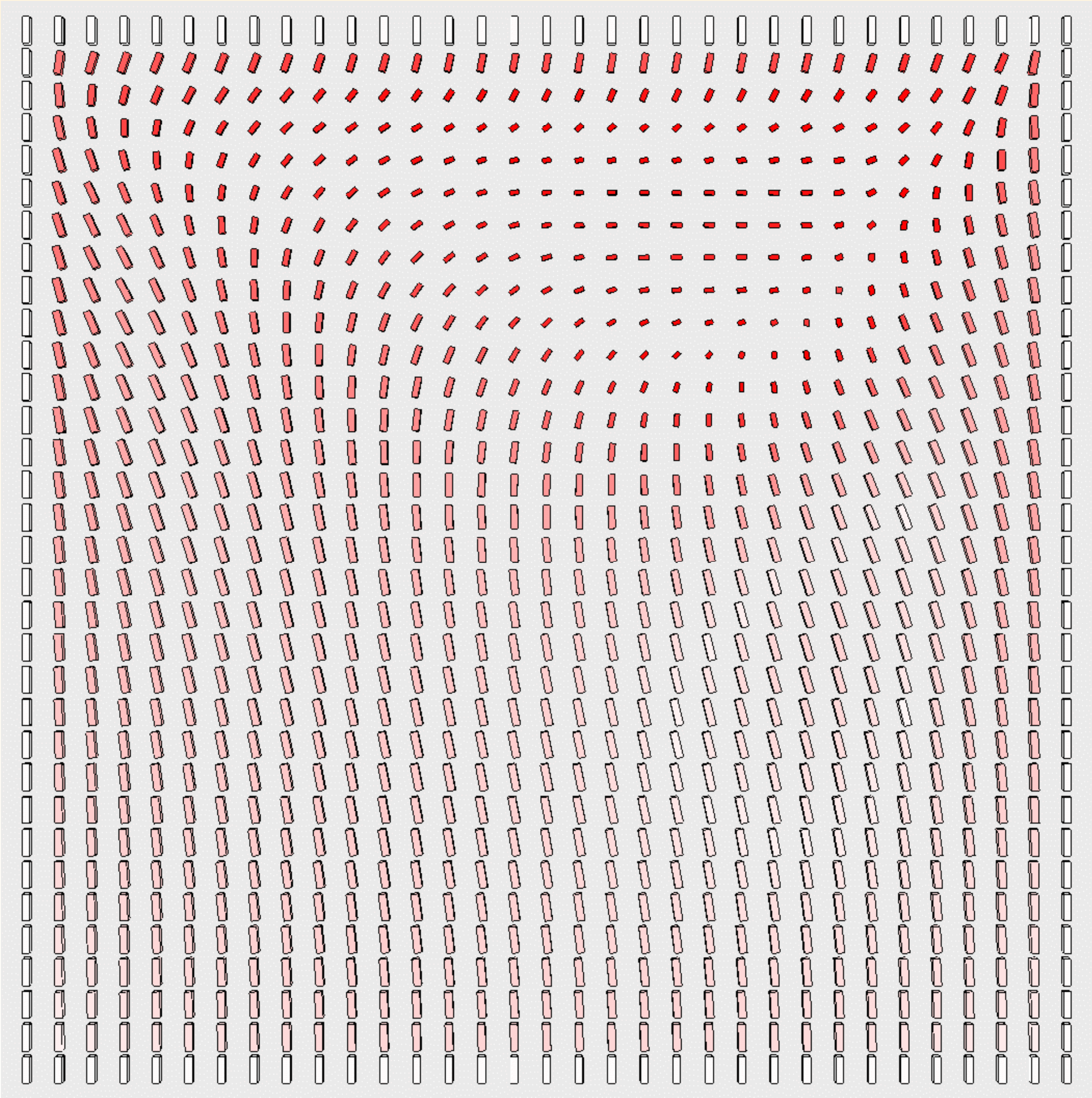
Initial Orientation



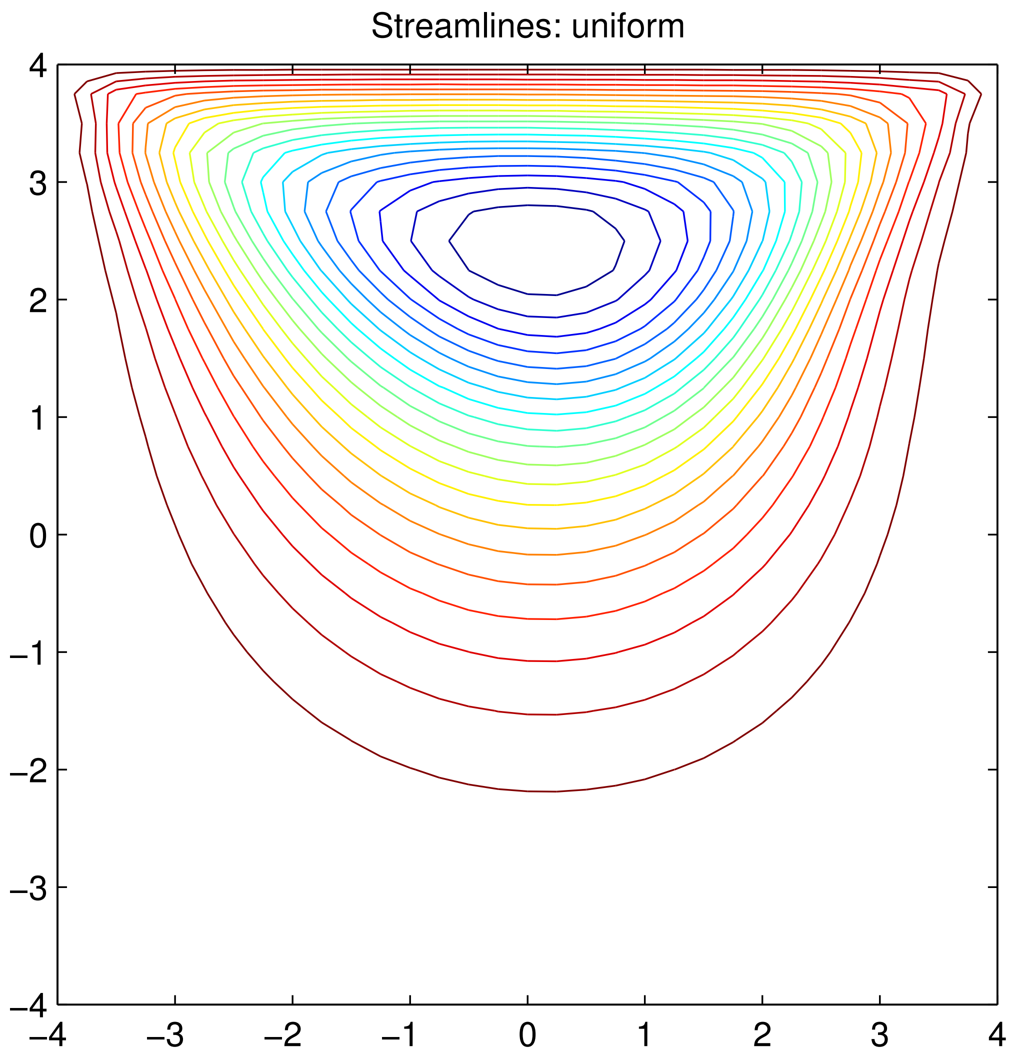
Initial Flow Field



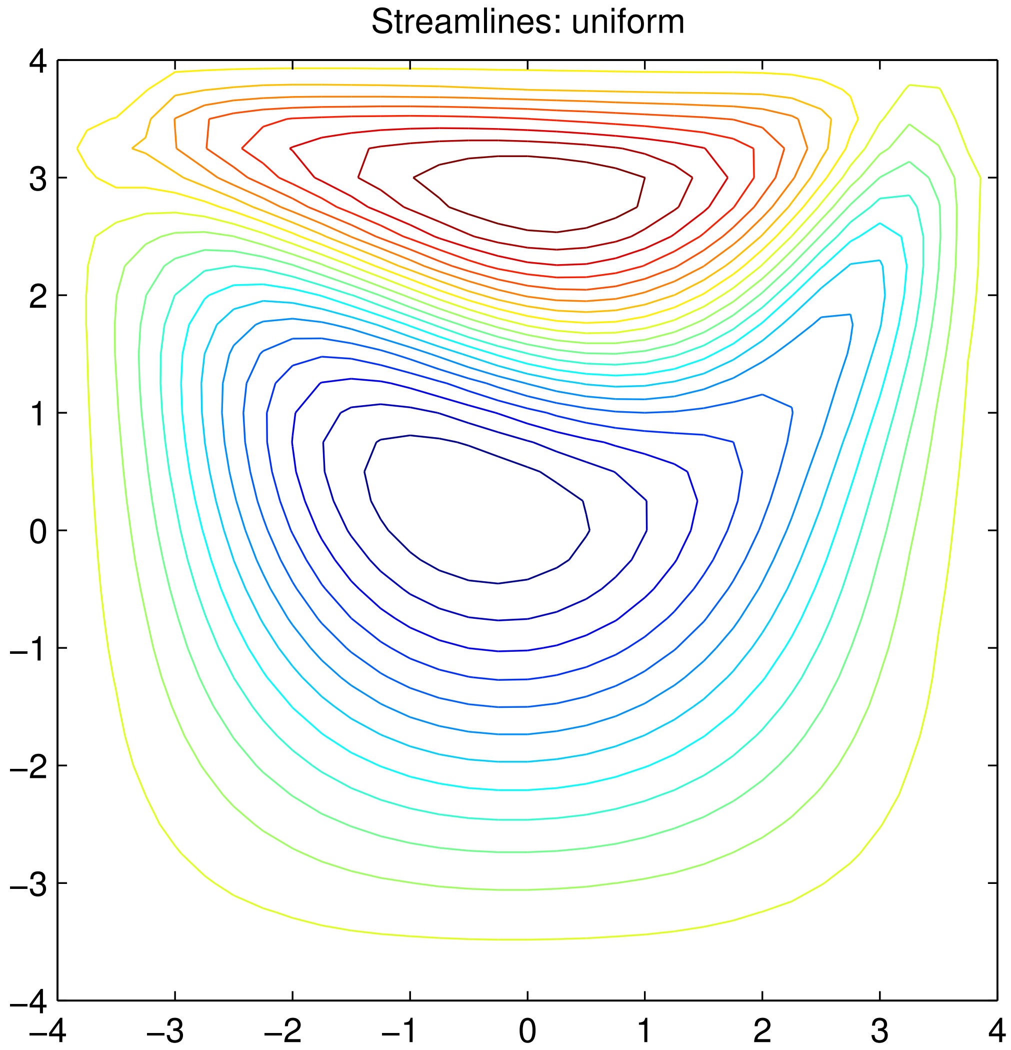
Later Orientation



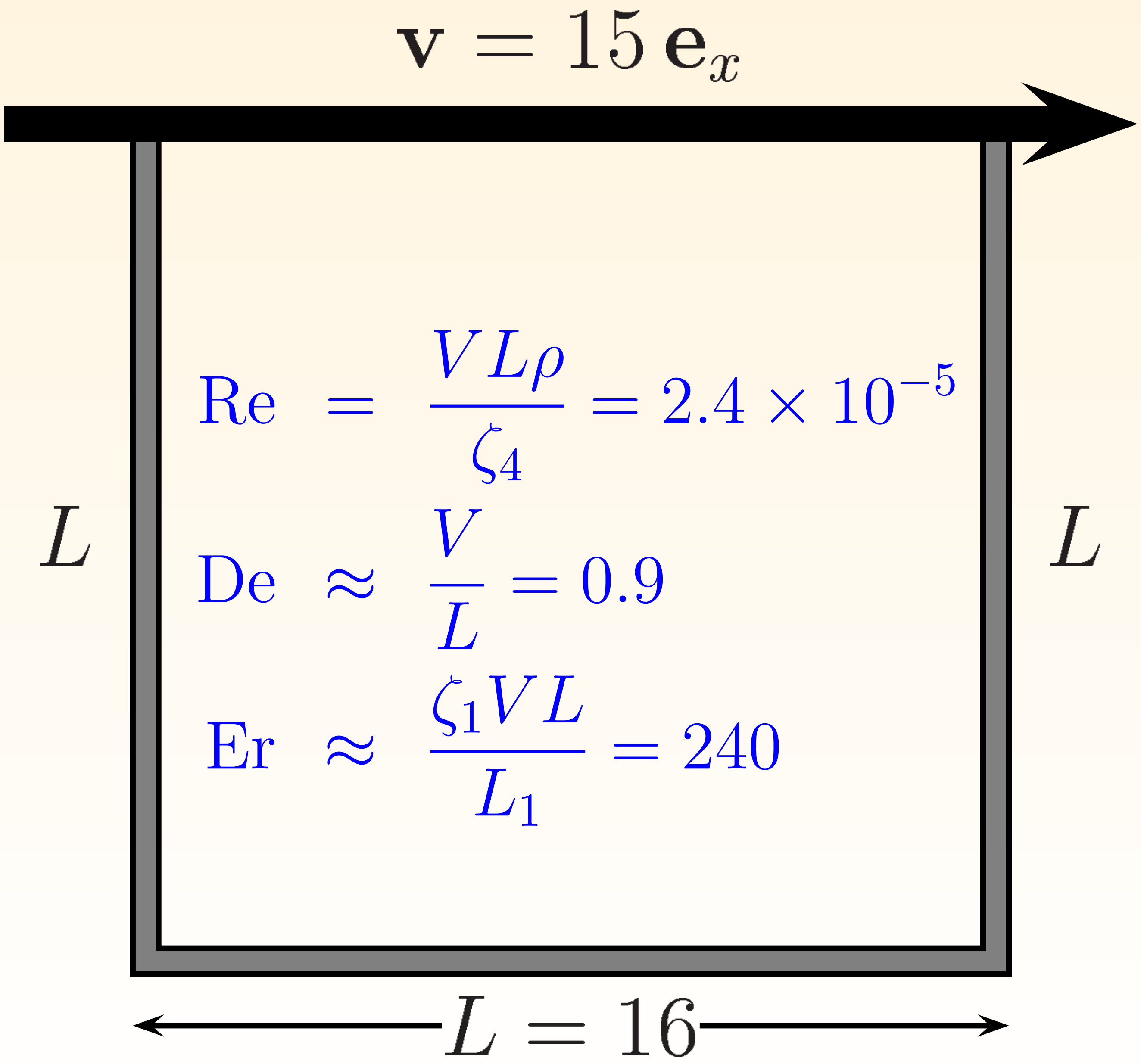
Later Flow Field



Flow Field Difference



Out of Plane Orientation

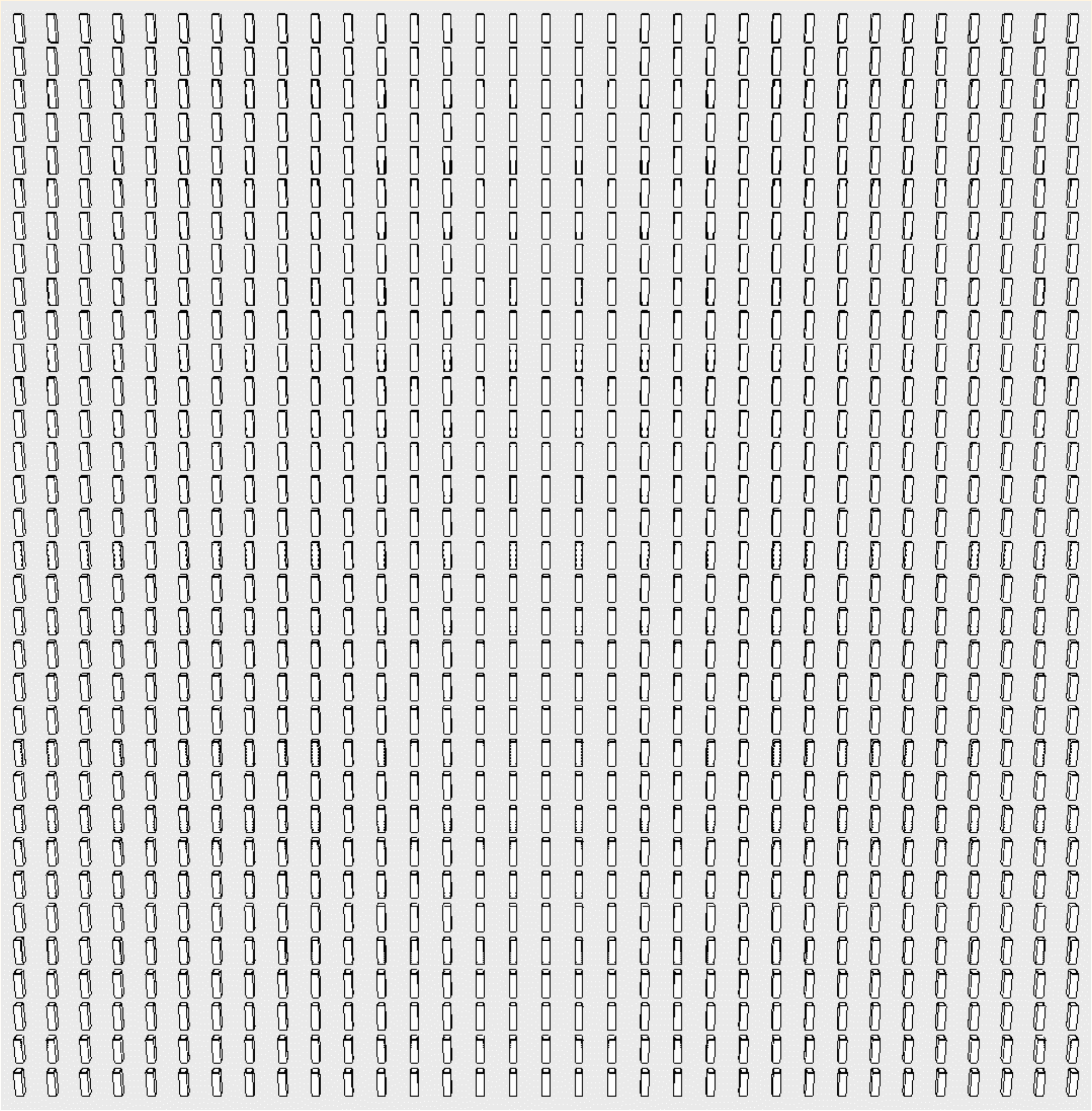


$$\mathrm{Re} = \frac{VL\rho}{\zeta_4} = 2.4 \times 10^{-5}$$

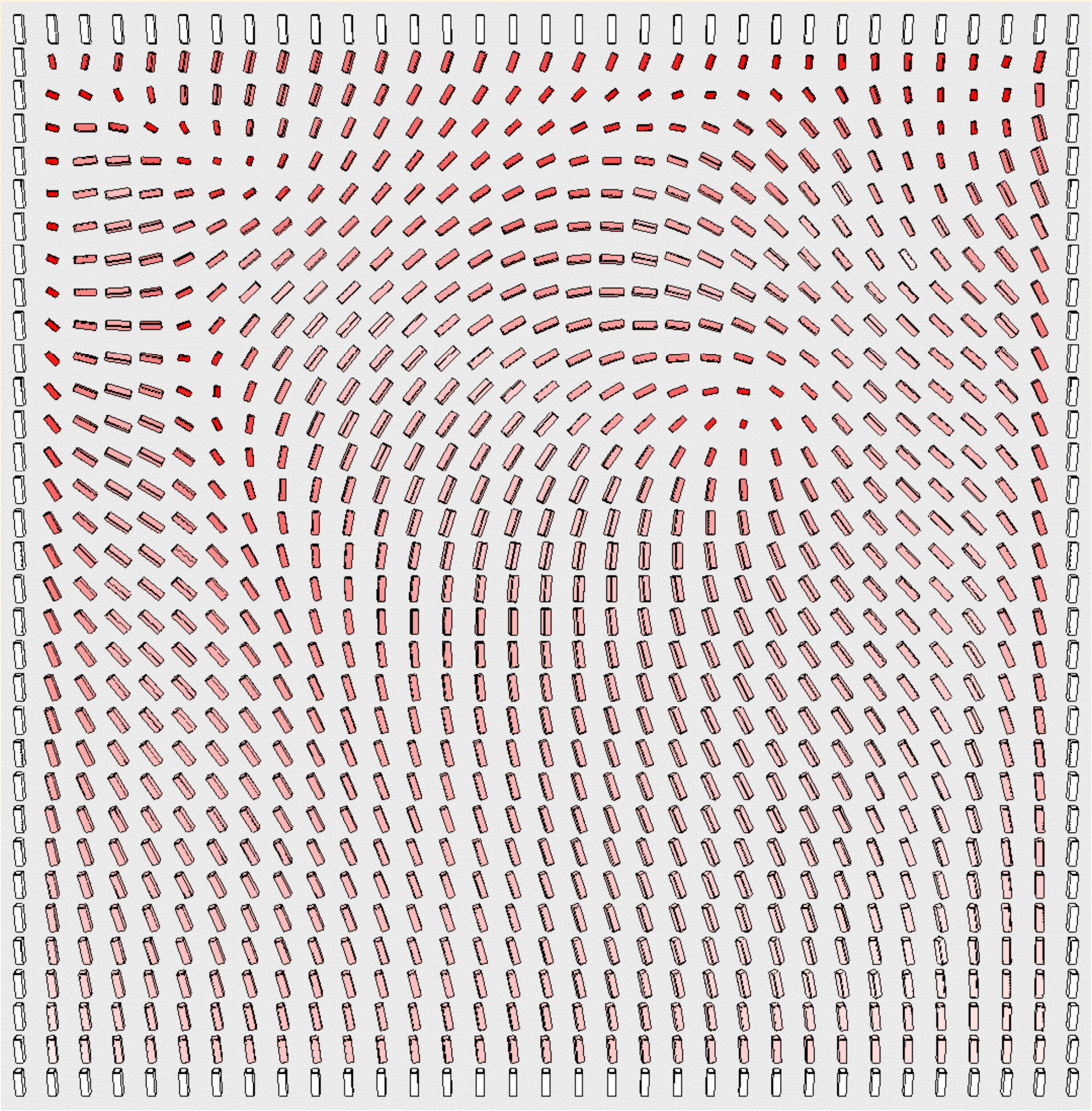
$$\mathrm{De} \approx \frac{V}{L} = 0.9$$

$$\mathrm{Er} \approx \frac{\zeta_1 V L}{L_1} = 240$$

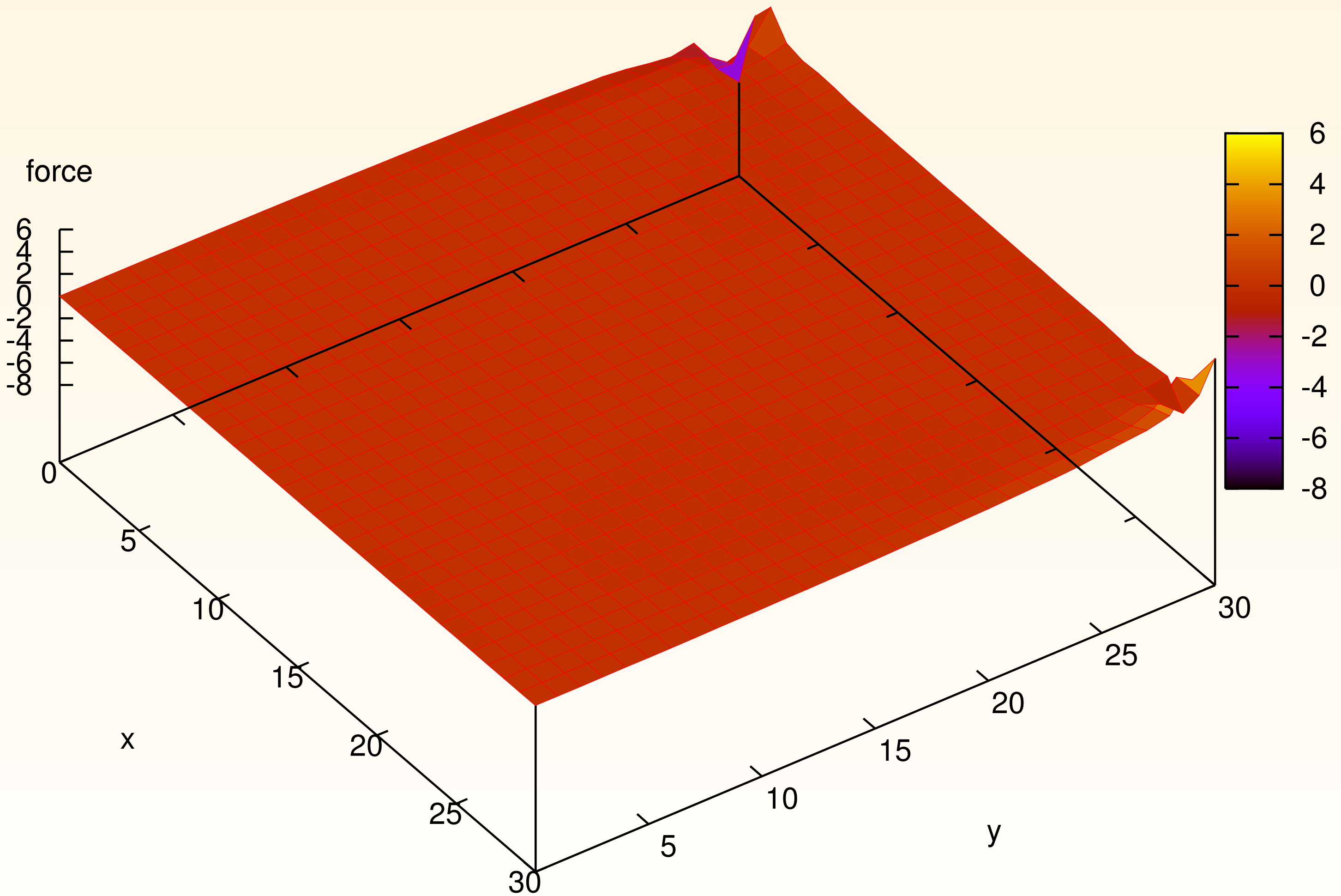
Initial Orientation



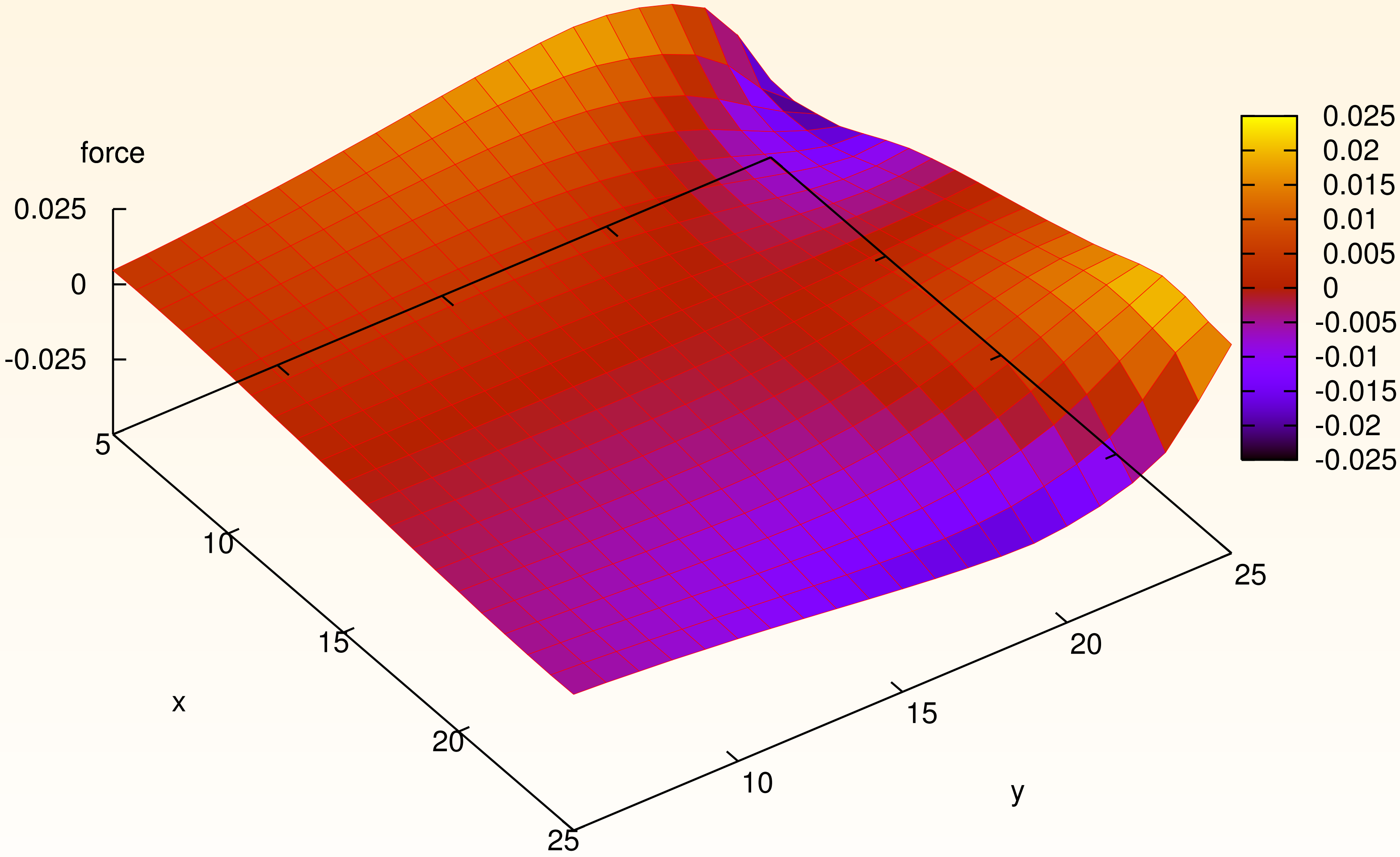
Later Orientation



Out of Plane Force



Out of Plane Force



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- A lot of work still needs to be done . . .