Computational Fluid Dynamics of Nematic Liquid Crystals Described by the Q-Tensor Model

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Overview

1. Equations for Flow and Orientation

2. Numerical Method

3. Lid Driven Cavity

Structure of Equations

$$\rho \dot{\boldsymbol{v}} = \operatorname{div} \mathbf{T}, \qquad \mathbf{T}(\mathbf{D}, \mathbf{Q}, \overset{\circ}{\mathbf{Q}}, \ldots)$$
$$\overset{\circ}{\mathbf{Q}} = \ldots \qquad (\mathbf{D}, \mathbf{Q}, \nabla \mathbf{Q})$$

$\mathbf{Q}$, $\overset{\circ}{\mathbf{Q}}$ alignment tensor and its co-rotational time derivative

$\mathbf{T}$ stress tensor

$\mathbf{D}$ symmetric part of the velocity gradient

Idea: Use the equation for the orientation to reduce the stress to a form that can be used in standard CFD packages!

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Time derivatives of the Q-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 $\mathbf{W} = \frac{1}{2}(\nabla \boldsymbol{v} - (\nabla \boldsymbol{v})^T)$

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Equations of Motion

With the free energy W and the dissipation R,

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

$$\frac{\partial R}{\partial \mathring{\mathbf{Q}}} = \operatorname{div} \frac{\partial W}{\partial \nabla \mathbf{Q}} - \frac{\partial W}{\partial \mathbf{Q}}$$

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

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Basic Model

Dissipation:

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

Free Energy:

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

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.

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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

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

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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

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

and

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

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

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Viscosities

With ($\approx$ MBBA)

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

$$\Longrightarrow$$

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

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

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

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

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

$$\mathbf{F} = L_1 \left(\mathbf{Q}(\Delta \mathbf{Q}) - (\Delta \mathbf{Q})\mathbf{Q} + \frac{\zeta_2}{\zeta_1} \Delta \mathbf{Q} - \nabla \mathbf{Q} \odot \nabla \mathbf{Q} \right) - \frac{\zeta_2}{\zeta_1} \boldsymbol{\Phi}$$

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Strategy

1. For a given orientation field $\mathbf{Q}$, solve Stokes equation with 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

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

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Dimensionless Equations

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

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

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

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Solving the Equations

- Orientation equation: finite difference scheme with explicit euler time discretisation
- Stokes equation: finite element iterative solver. Matlab package using MINRES solver with multigrid preconditioning
  http://www.cs.umd.edu/~elman/ifiss.html
  (Incompressible Flow & Iterative Solver Software Version 2.2)

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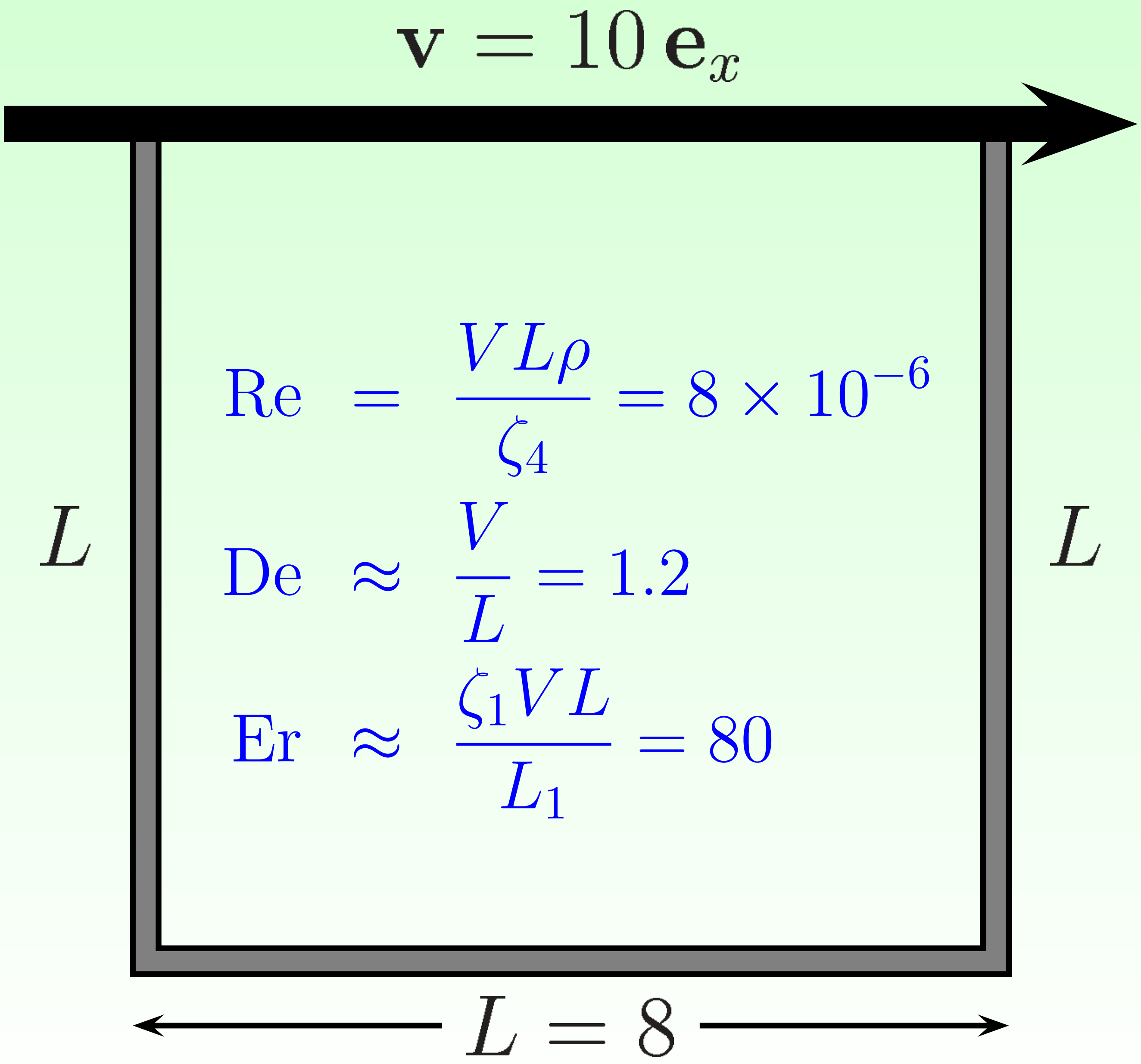
Lid Driven Cavity

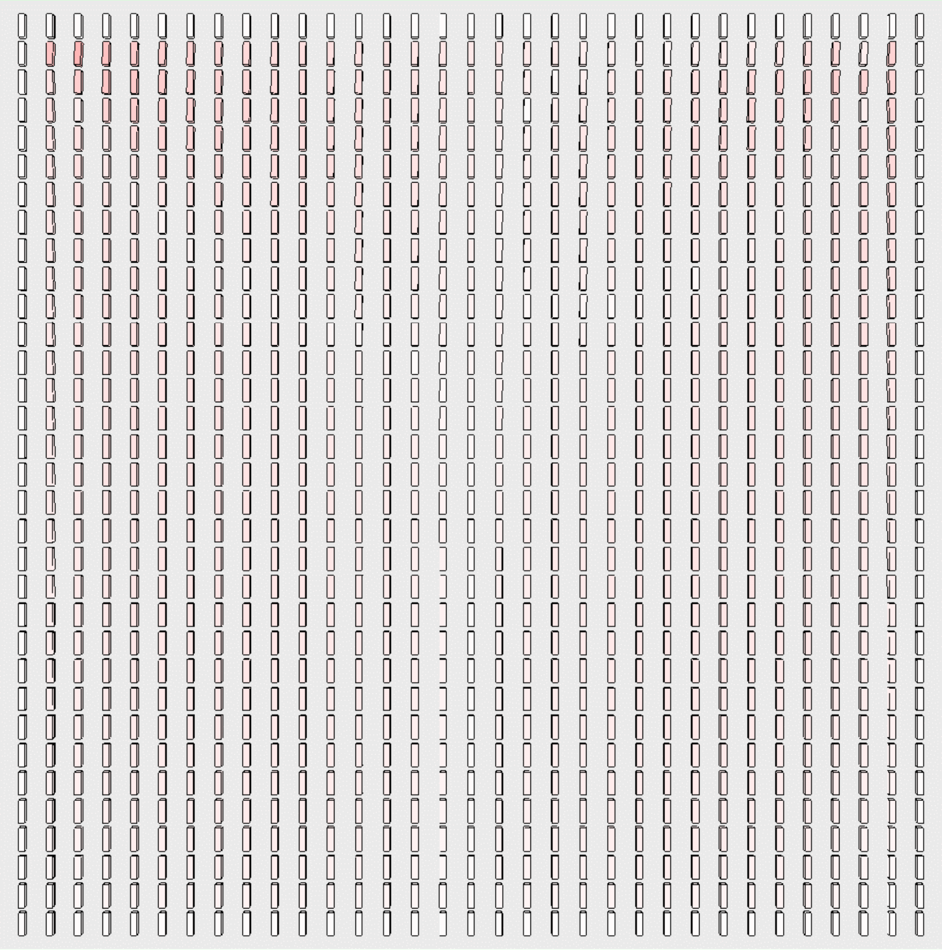


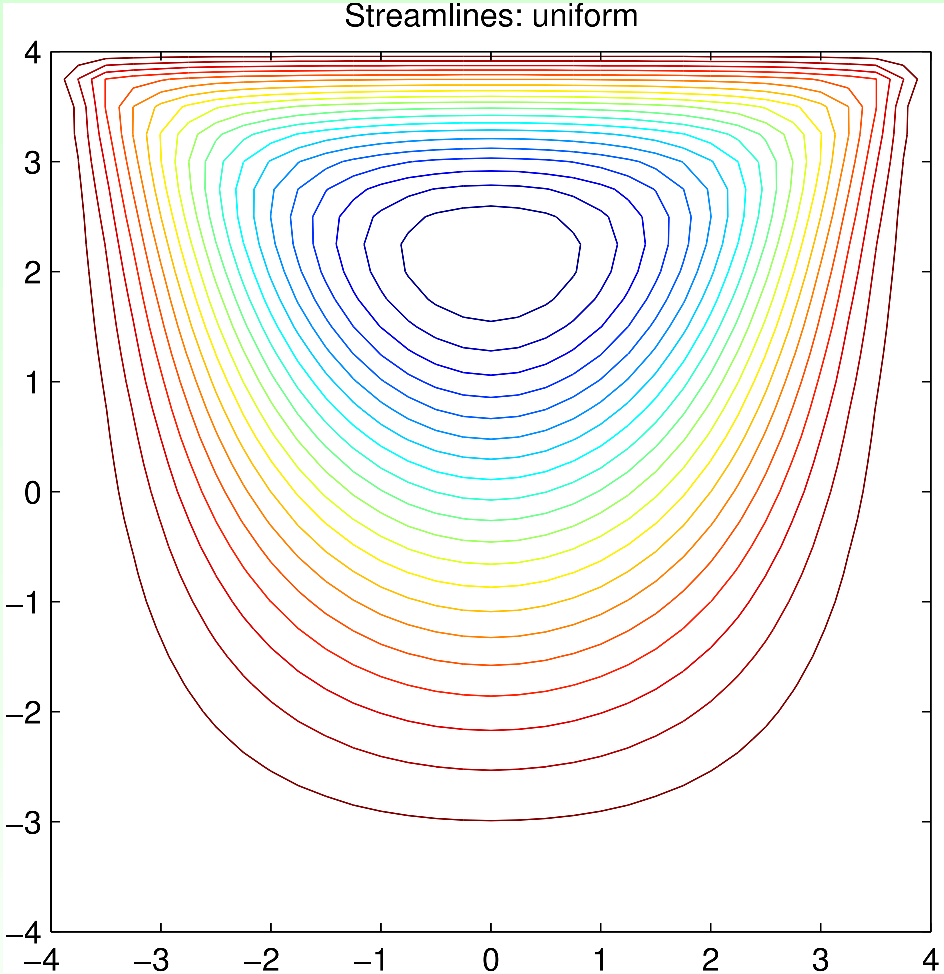
$$\mathrm{Re} = \frac{VL\rho}{\zeta_4} = 8 \times 10^{-6}$$

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

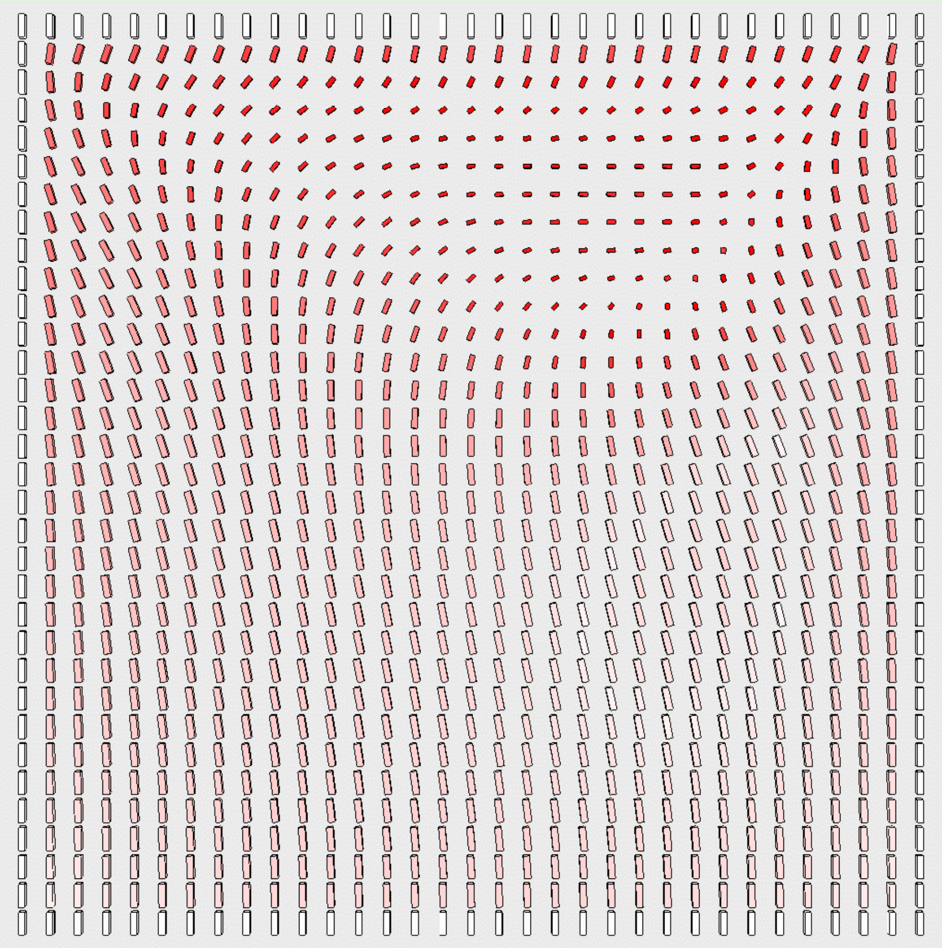
$$\mathrm{Er} \approx \frac{\zeta_1 V L}{L_1} = 80$$

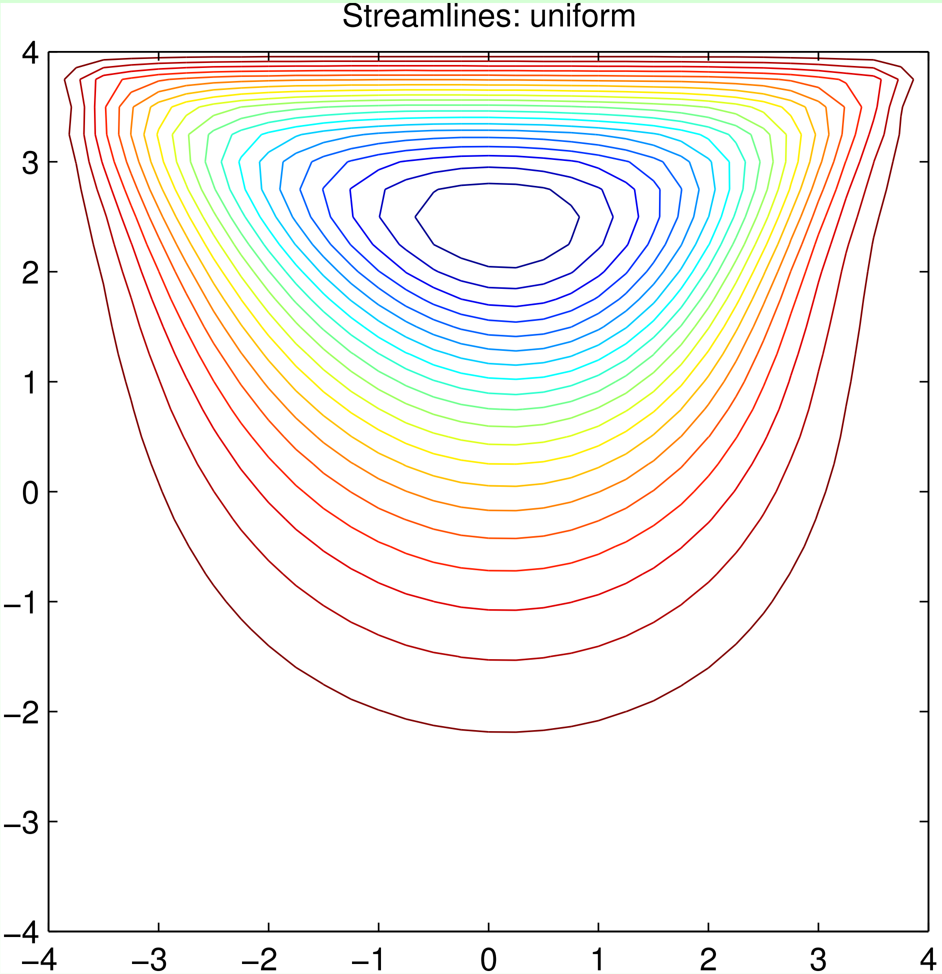
Initial Orientation and Flow Field



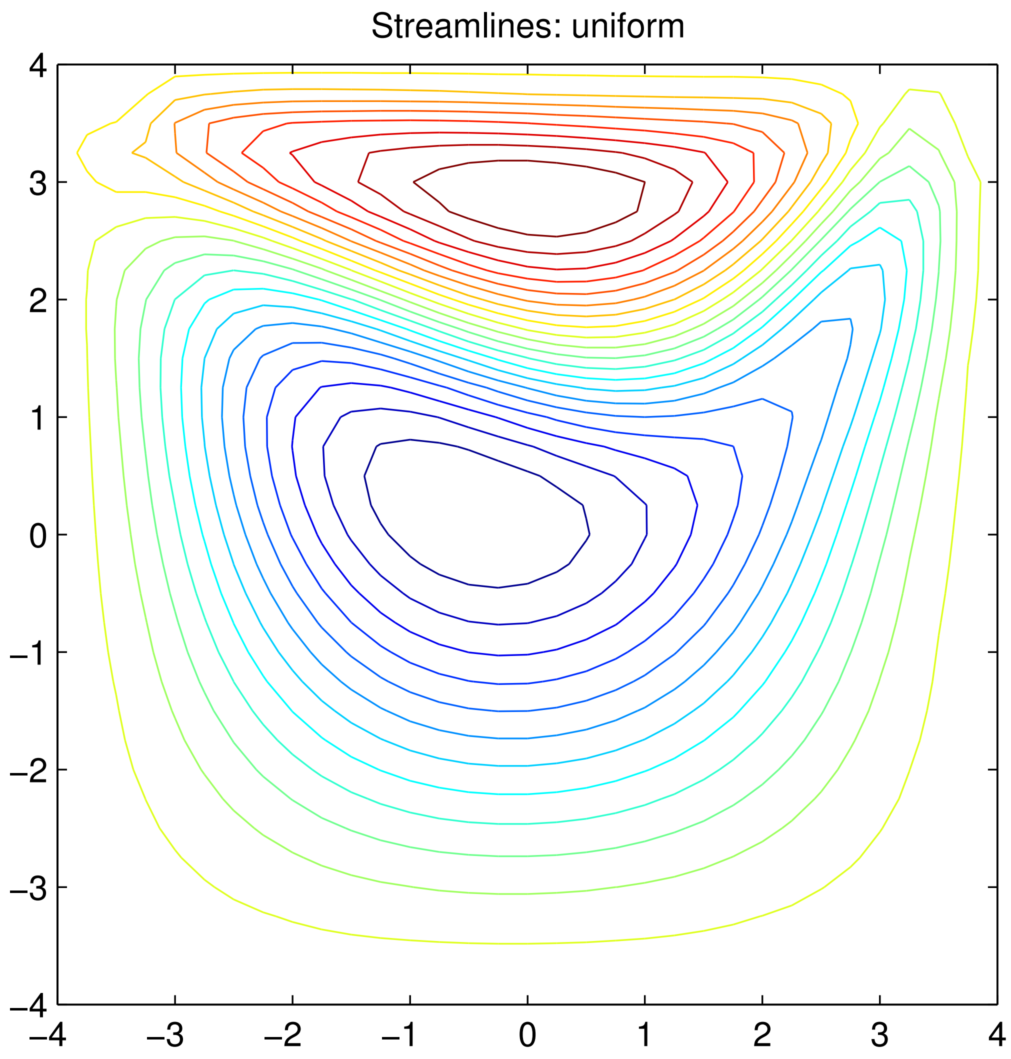


Later Orientation and Flow Field

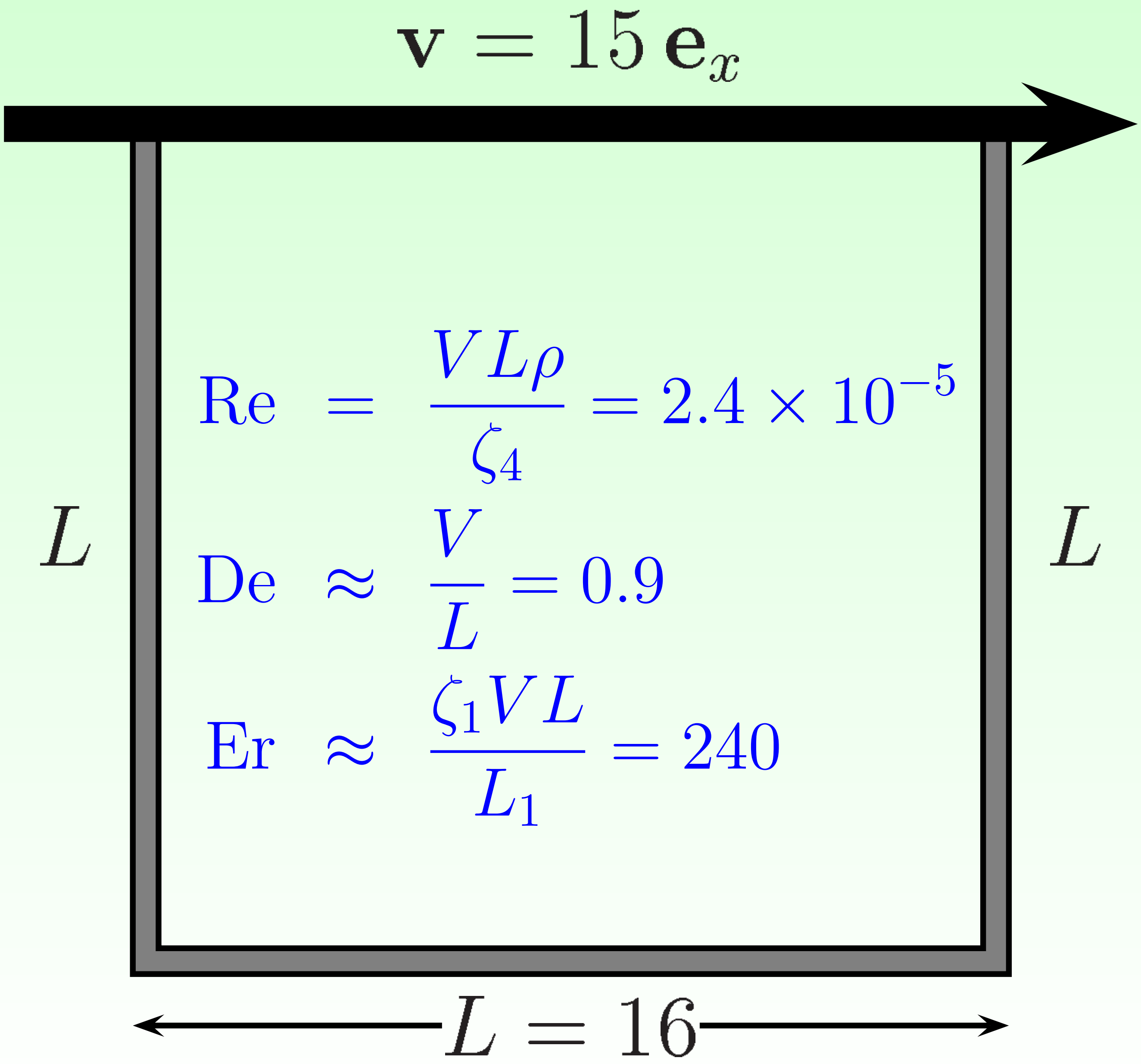




Flow Field Difference



Out of Plane Orientation

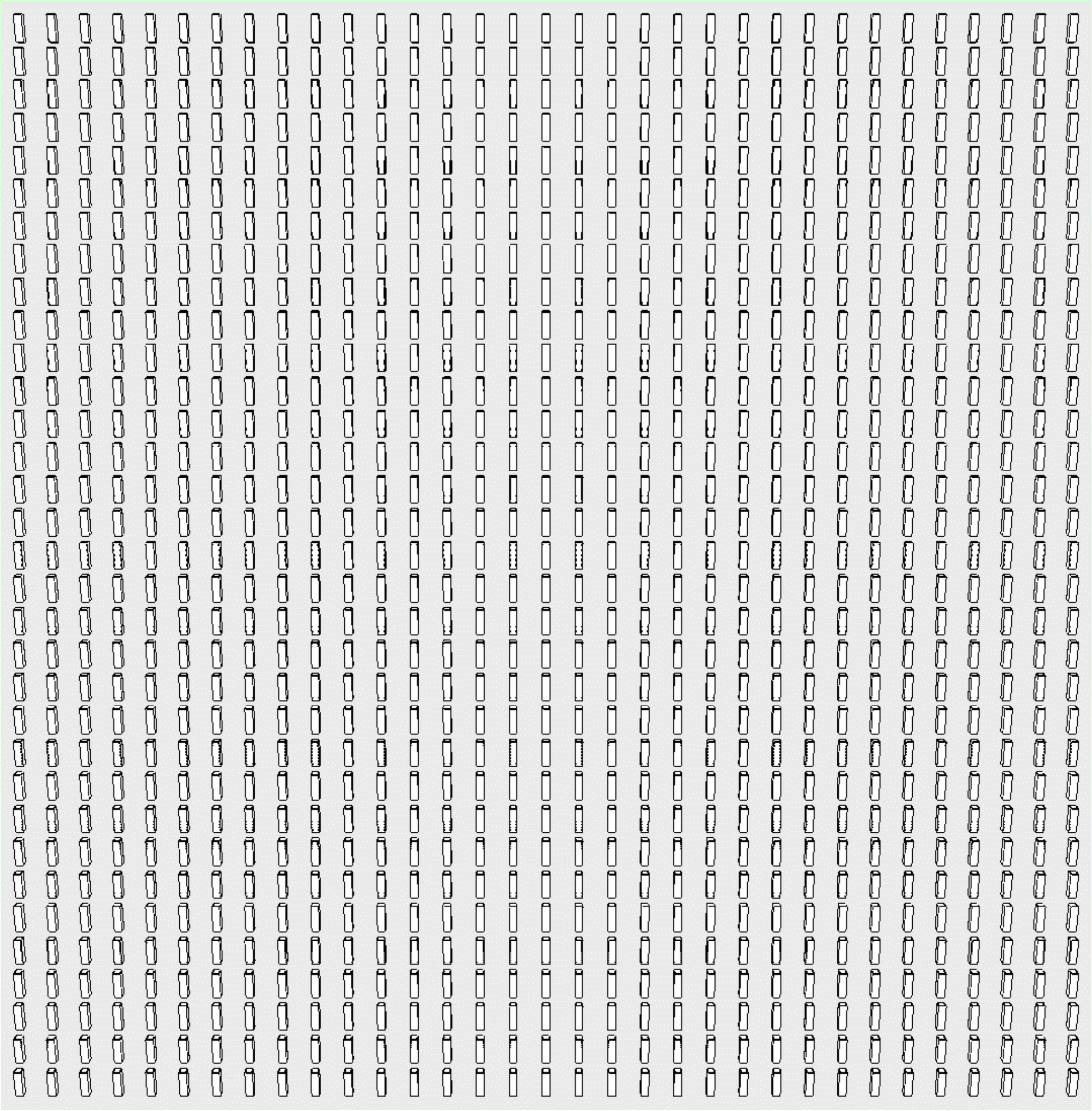


$$\mathrm{Re} = \frac{VL\rho}{\zeta_4} = 2.4 \times 10^{-5}$$

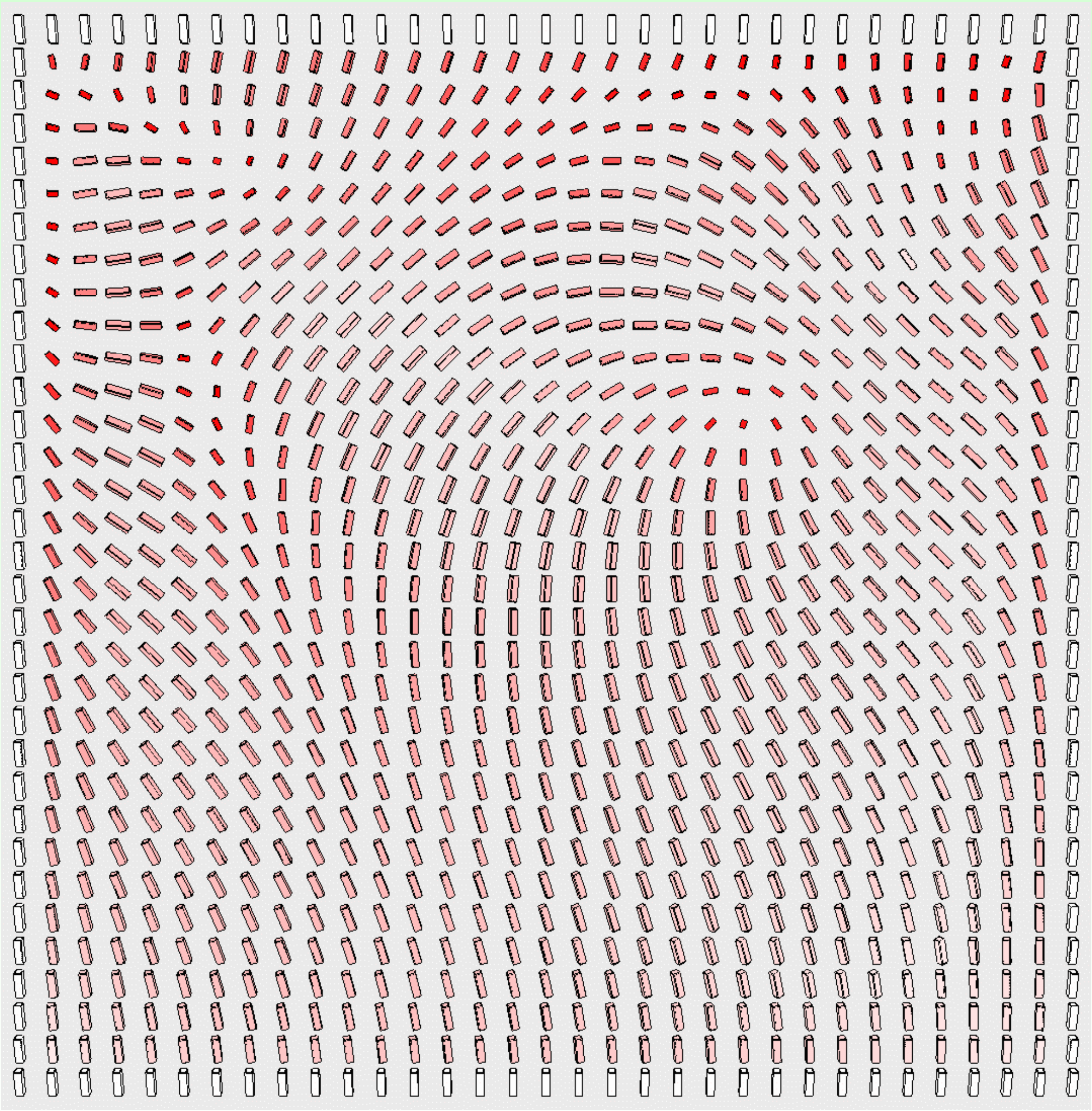
$$\mathrm{De} \approx \frac{V}{L} = 0.9$$

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

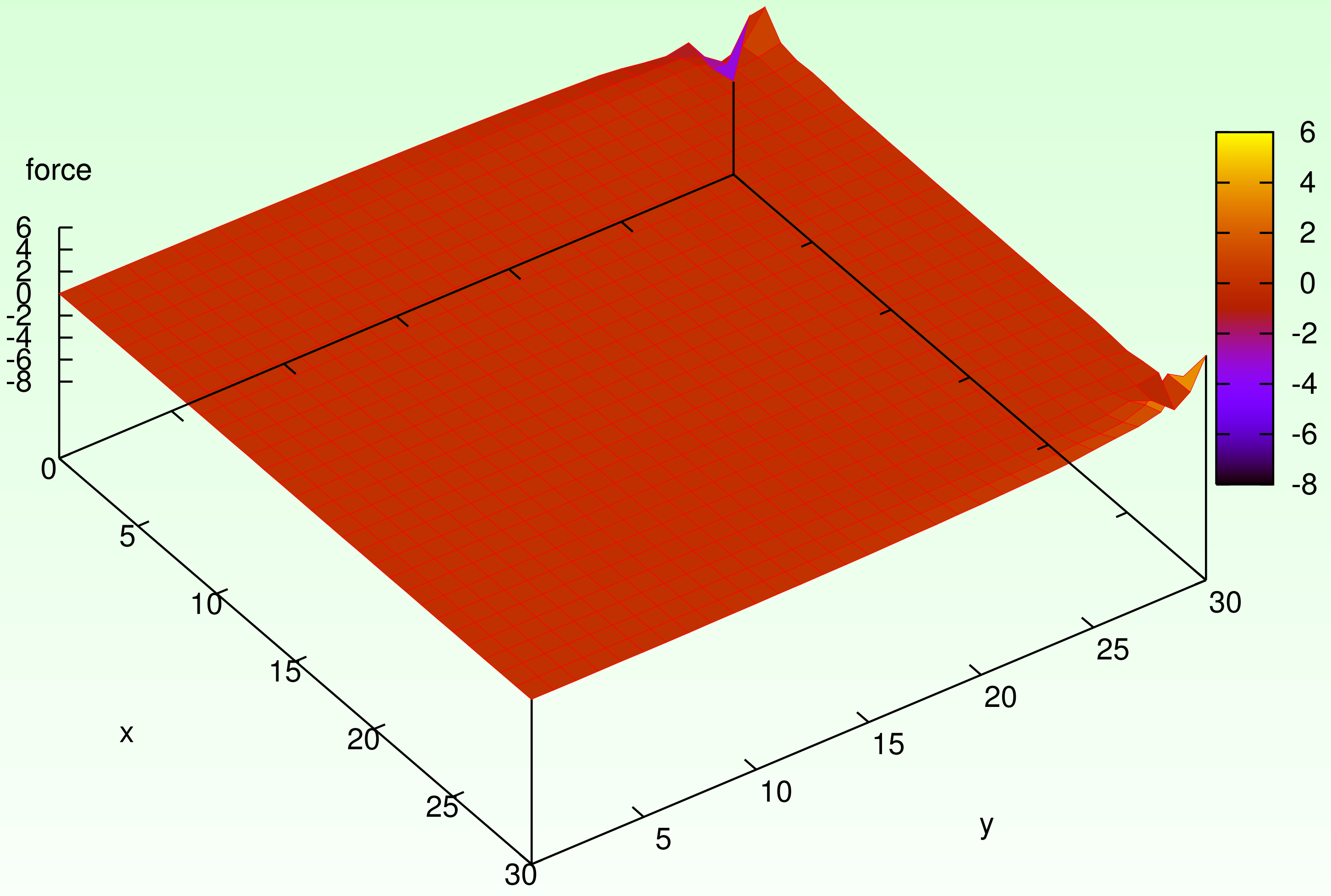
Initial Orientation



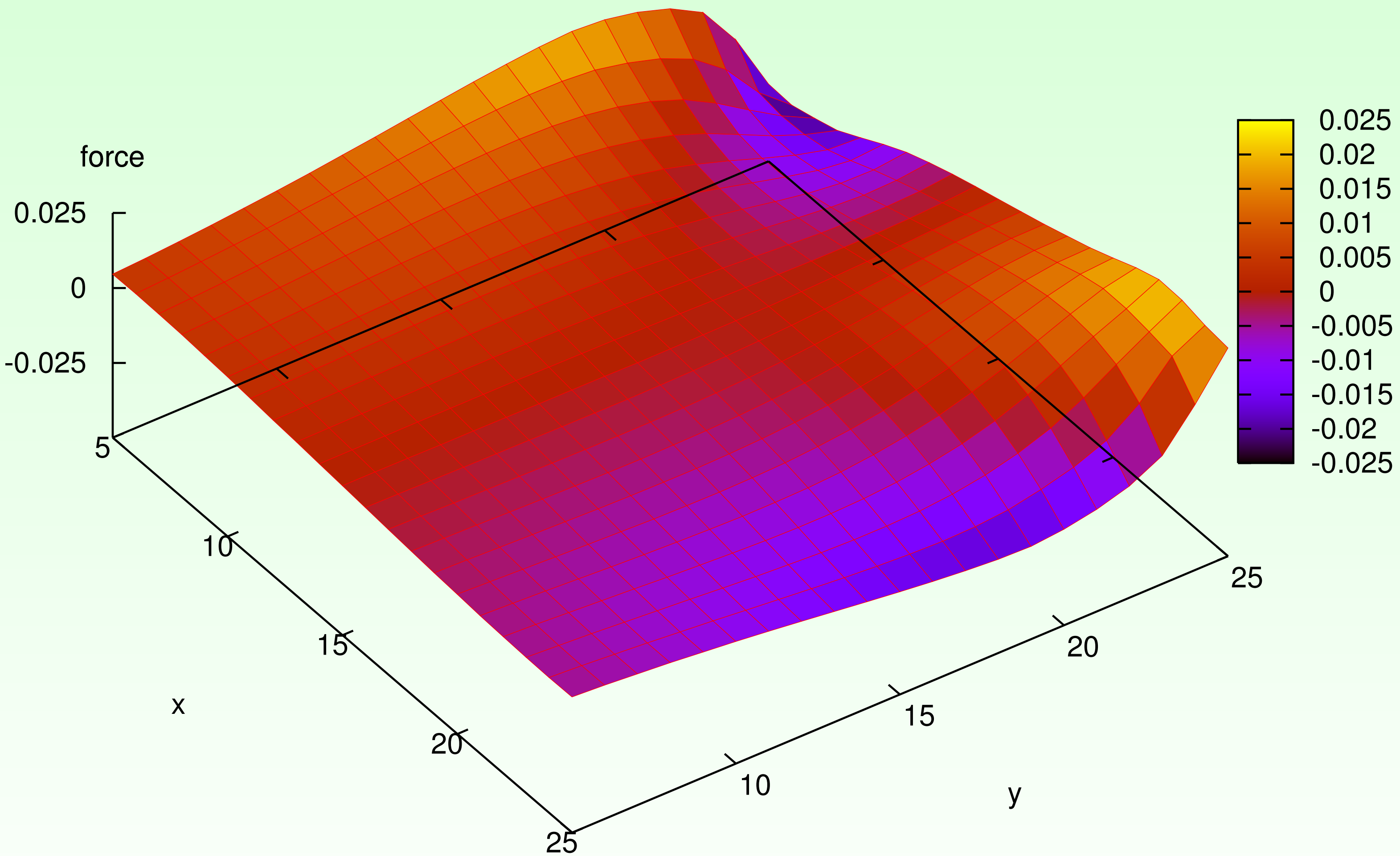
Later Orientation



Out of Plane Force



Out of Plane Force



Ericksen-Leslie-Parodi !?

The same method works in principle, but

- The Lagrange parameter needed for $\boldsymbol{n} \cdot \boldsymbol{n} = 1$ gives trouble
- $\alpha_1 = 0$ (which is fine)
- $\gamma_2^2 = \gamma_1 \gamma_3 \quad \rightarrow$ unrealistic material coefficients

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Summary

- Adding orientational order to Computational Fluid Dynamics can be very cheap!
- Non-linear effects even for ‘linear’ flow (low Reynolds numbers) :
  - Non-symmetrical flow profile
  - 2-D flow not stable
- Future work:
  - 3-D flow and orientation
  - Use of co-deformational time derivative allows four independent viscosity coefficients

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