IFISS : A Computational Laboratory for Investigating Incompressible Flow Problems

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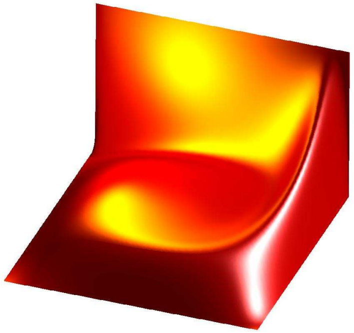


IFISS

Incompressible **F**low & **I**terative **S**olver **S**oftware

- download from

  `www.manchester.ac.uk/ifiss`
  `www.cs.umd.edu/∼elman/ifiss`

- open-source software package run under MATLAB or GNU OCTAVE

Incompressible Flow & Iterative Solver Software

An open-source software package

Summary

IFISS is a graphical package for the interactive numerical study of incompressible flow problems which can be run under Matlab or Octave. It includes algorithms for discretization by mixed finite element methods and a posteriori error estimation of the computed solutions. The package can also be used as a computational laboratory for experimenting with state-of-the-art preconditioned iterative solvers for the discrete linear equation systems that arise in incompressible flow modelling.

Key Features

Key features include

- implementation of a variety of mixed finite element approximation methods;
- automatic calculation of stabilization parameters where appropriate;
- a posteriori error estimation for steady problems;
- a range of state-of-the-art preconditioned Krylov subspace solvers ;
- built-in geometric and algebraic multigrid solvers and preconditioners;
- fully implicit self-adaptive time stepping algorithms;
- useful visualization tools.

The developers of the IFISS package are David Silvester (School of Mathematics, University of Manchester), Howard Elman (Computer Science Department, University of Maryland), and Alison Ramage (Department of Mathematics and Statistics, University of Strathclyde).

The IFISS logo represents the solution of the *double glazing* convection-diffusion problem. It can be reproduced in IFISS via the function **ifisslogo**.

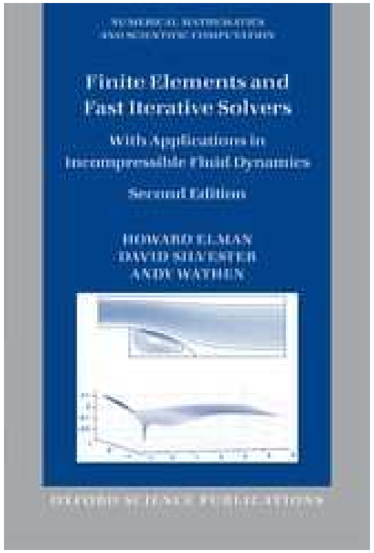
This webpage is based on a CSS template from Free CSS Templates.

Motivation and Philosophy

- Numerical analysis research is frequently motivated by numerical experiments: "proof by MATLAB" often comes before any formal analytic results.
- Carrying out investigative numerical experiments helps students learn how to formulate hypotheses, design simple experiments to test them and interpret the resulting data.
- A hands-on approach often leads to better understanding.
- The computational laboratory plays just as important a role in modern mathematics as physical laboratories do in physics, chemistry, biology and engineering.

Development Highlights

version		date
1.0	created for Utrecht workshop	1997
1.3	MG solvers/preconditioners added	1998
2.0	Elman/Silvester/Wathen monograph	2005
2.2	TOMS paper	2007
3.2	SIREV paper	2012
3.3	final release	2014


Finite Elements and
Fast Iterative Solvers
With Applications in
Incompressible Fluid Dynamics
Second Edition
HOWARD ELMAN
DAVID SILVESTER
ANDY WATHEN

Elman, Silvester and Wathen

Finite Elements and Fast Iterative Solvers: with applications in incompressible fluid dynamics

2nd edition, Oxford University Press, 2014.

Overview

Four underlying PDEs on two-dimensional domains:

- Diffusion equation

$$\nabla^2 u = f$$

- Convection-Diffusion equation

$$-\epsilon\nabla^2 u + w \cdot \nabla u = f$$

- Stokes equations

$$\begin{aligned} -\nabla^2 u + \text{grad}\, p &= f \\ -\text{div}\, u &= 0 \end{aligned}$$

- Navier-Stokes equations

$$\begin{aligned} -\nu\nabla^2 u + (u \cdot \text{grad})\, u + \text{grad}\, p &= f \\ -\text{div}\, u &= 0 \end{aligned}$$

Test problems

- Over thirty built-in test problems with driver routines.
- Most involve steady-state versions of the four key PDEs.
- Remaining problems associated with the heat equation and time-dependent versions of the convection-diffusion equation, the Navier-Stokes equations and their Boussinesq flow combination.
- New problems on PDE-constrained optimization (Poisson control problems).

  Pearson and Wathen NLAA 19 (2012)

Two Main Components

Finite element discretisations

- Bilinear/biquadratic elements on rectangles
- Streamline upwinding for convection-diffusion equation
- Mixed finite elements for Stokes/Navier-Stokes equations with stable and stabilised elements
- A posteriori error estimation

Iterative solution of discrete (linearised) systems

- Preconditioned Krylov subspace methods

PCG MINRES GMRES

BiCGStab(ℓ) IDR(s)

Preconditioners

- Jacobi, Incomplete Cholesky, ILU
- Geometric multigrid (also available as a solver)

  Ramage JCAM 101 (1999)
- Algebraic multigrid (HSL_MI20)

  Boyle, Mihajlovic and Scott IJNME 82 (2010)
- Block preconditioners for saddle point problems

  Silvester and Wathen SINUM 31 (1994)
- Pressure convection-diffusion preconditioning

  Silvester et al. JCAM 128 (2001), Kay et al. SISC 24 (2002)
- Least squares commutator preconditioning

  Elman SISC 20 (1999), Elman et al. SISC 27 (2006)

Other Key Features

- several problem domains square, L-shaped, step
- graphical displays grid, solution, error estimate
- user access to data and problem structure
- full user access to code
- user can change problem features:
  - domain
  - boundary conditions
  - solvers

Example 1: Convection-Diffusion

$$-\epsilon\nabla^2 u + w\cdot\nabla u = f$$

- Galerkin FEM

$$\epsilon(\nabla u_h, \nabla v_h) + (w\cdot\nabla u_h, v_h) = (f, v_h) \quad \forall v_h \in V_h$$

- Petrov-Galerkin FEM (streamline diffusion)

$$\begin{aligned}\epsilon(\nabla u_h, \nabla v_h) \quad &+ \quad (w\cdot\nabla u_h, v_h) + \frac{\delta h}{||w||}(w\cdot\nabla u_h, w\cdot\nabla v_h) \\ &= \quad (f, v_h) + \frac{\delta h}{||w||}(f, w\cdot\nabla v_h) \quad \forall v_h \in V_h\end{aligned}$$

- parameter δ generated automatically

Fischer, Ramage, Silvester and Wathen BIT 38 (1998)

Elman and Ramage SINUM 40 (2002), Math. Comp. 72 (2003)

Problem Specification

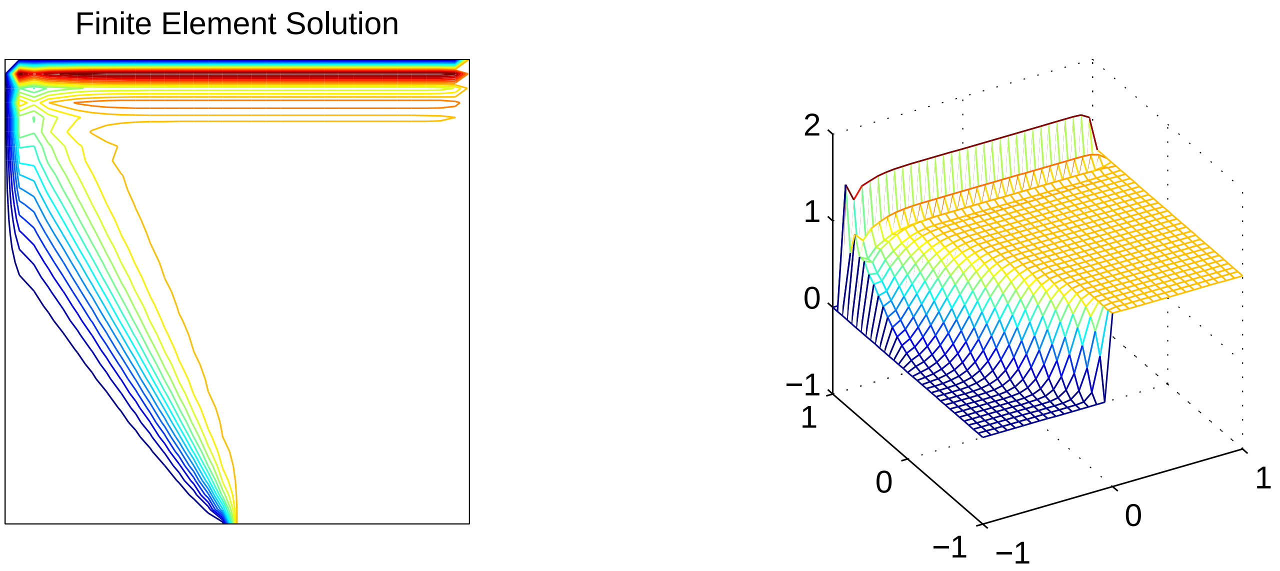
- square domain
- constant wind at angle of 30° to the left of vertical

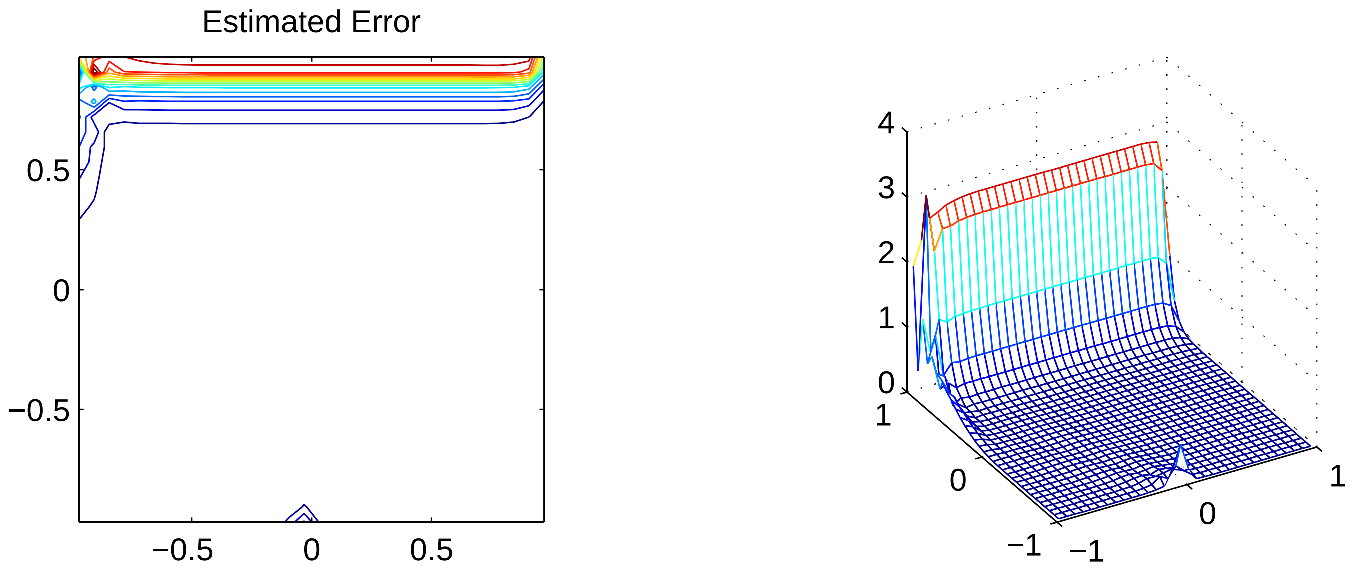
$$\mathbf{w} = \left(-\sin\tfrac{\pi}{6},\ \cos\tfrac{\pi}{6}\right)$$

- Dirichlet boundary conditions:
  - 0 on left and top boundaries
  - 1 on the right boundary
  - jump discontinuity (from 0 to 1) on the bottom boundary at (0,-1)
- solution features:
  - exponential boundary layer near the top boundary
  - internal layer as discontinuity smeared by the presence of diffusion

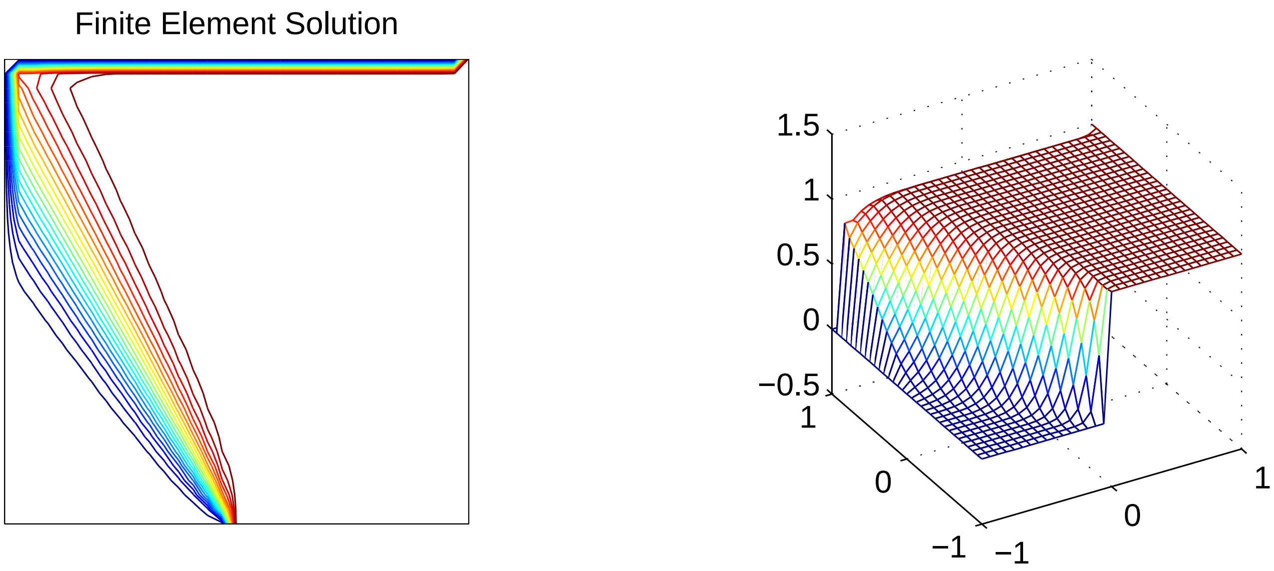
```
specification of reference convection-diffusion problem.
choose specific example
 1 Constant vertical wind
 2 Vertical wind, characteristic layers
 3 Constant wind @ 30 degree angle
 4 Recirculating wind
:  3
Grid generation for unit square domain.
grid parameter:  3 for underlying 8x8 grid (default is 16x16) :  5
uniform/stretched grid (1/2) (default is uniform) :  1
[0,1] or [-1,1] square (enter 1/2) (default is [-1,1]) :  2
setting up Q1 convection-diffusion matrices...  done
system matrices saved in square_cd_nobc.mat ...
viscosity parameter (default 1/200) :  1/100
plotting element data...  done
maximum element Peclet number is 3.608439e+00
SUPG parameter (default is optimal) :  0
setting up Q1 SUPG stabilisation matrix...  done
system saved in square_cd.mat ...
solving linear system ...  done
linear system solved in 7.031e-03 seconds
computing Q1 element flux jumps...  done
computing local error estimator...  done
estimated global error (in energy):  1.087025e+01
plotting solution and estimated errors...  done
```

Galerkin discretisation

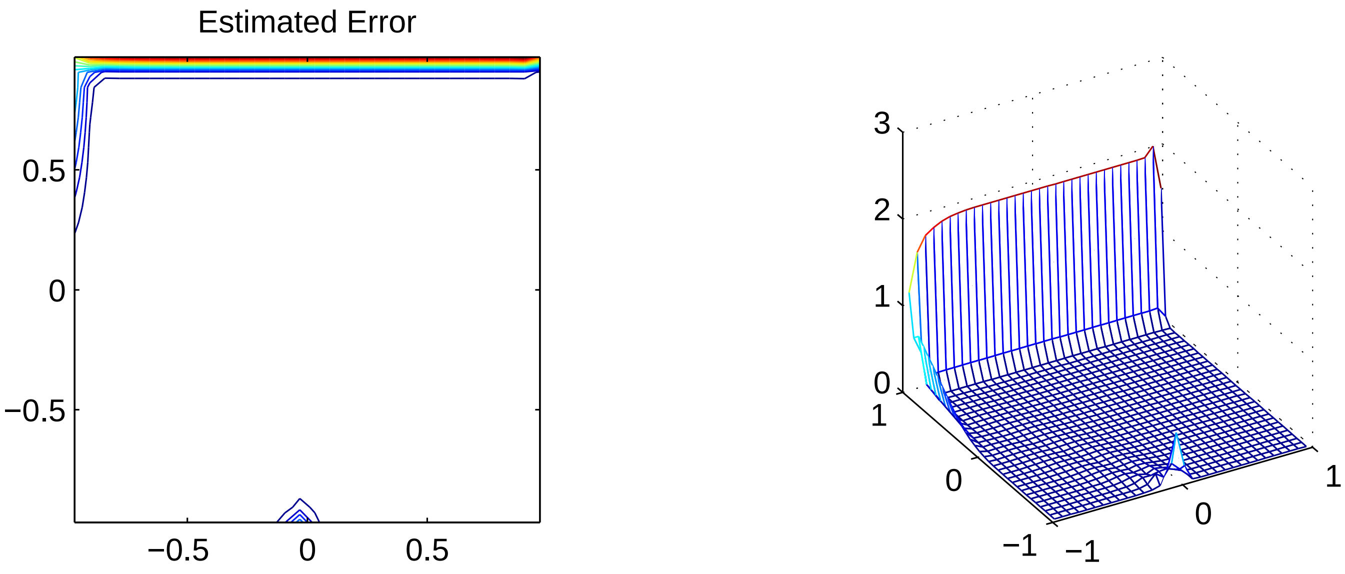

Finite Element Solution


Estimated Error

Petrov-Galerkin discretisation



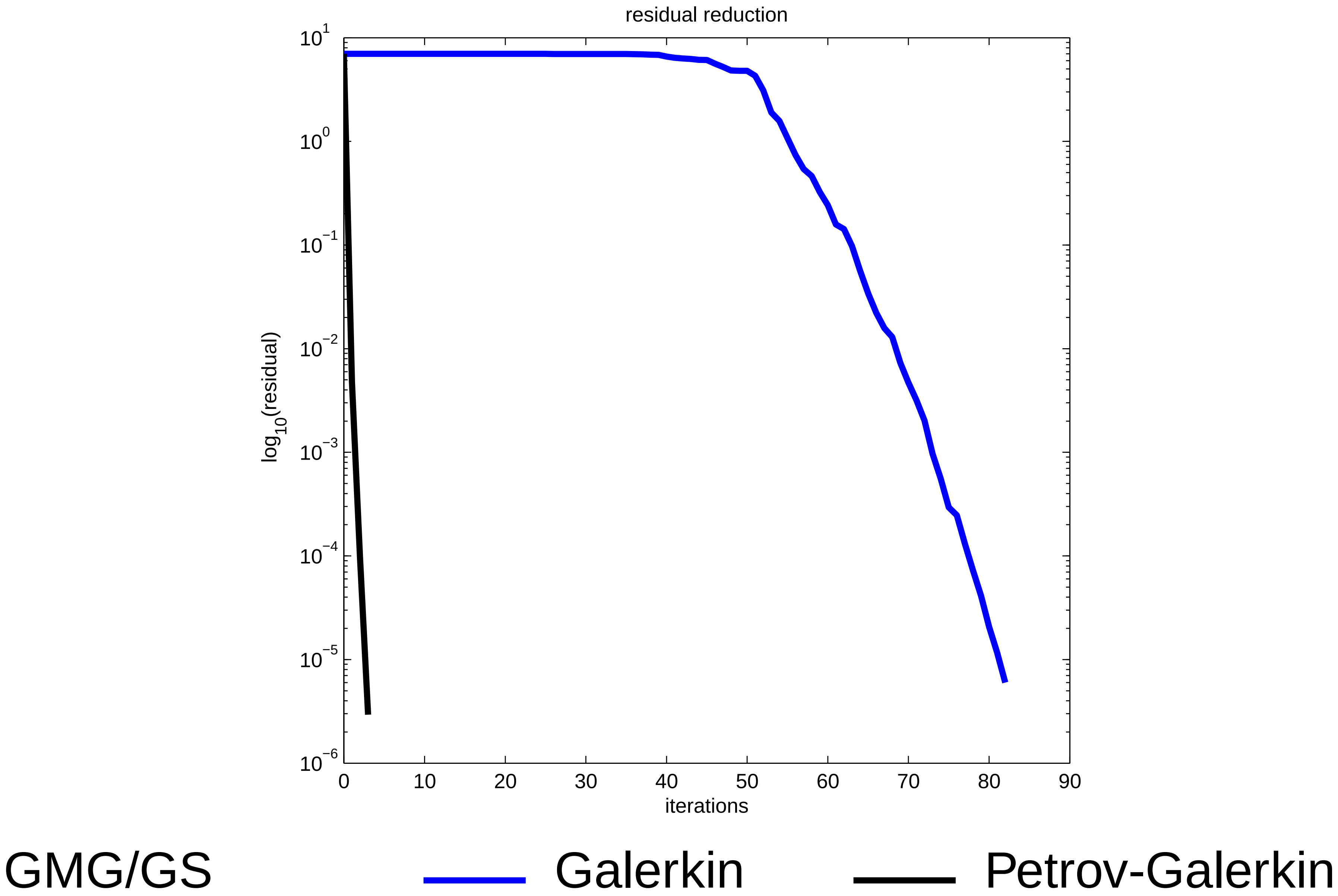
Finite Element Solution



Estimated Error

```
discrete convection-diffusion system ...
GMRES/Bicgstab(l)/IDR(s) 1/2/3 (default GMRES) :
stopping tolerance?  (default 1e-6) :
maximum number of iterations?  (default 100) :
preconditioner:
 0 none
 1 diagonal
 2 incomplete LU
 3 geometric multigrid
 4 algebraic multigrid
default is AMG : 3
compute / load MG data?  1/2 (default 1) :
Setting up MG data ...done
Jacobi / Gauss-Seidel / ILU smoother?  1/2/3 (default is Gauss-Seidel) :
point / line Gauss-Seidel?  1/2 (default is line) :
number of Gauss-Seidel directions?  1/2/3/4 (default is 2) :
number of pre-smoothing steps?  (default is 1) :
number of post-smoothing steps?  (default is 1) :
GMRES iteration ...  convergence in 3 iterations
 k log10($||r_k||/||r_0||$)
 0 0.0000
 1 -3.6484
 2 -5.5940
 3 -7.4461
Bingo!
```

Sample Results: Convection-Diffusion



Example 2: Stokes Flow

$$-\Delta u + \nabla p = f, \qquad \nabla \cdot u = 0$$

- classical test problem used in fluid dynamics

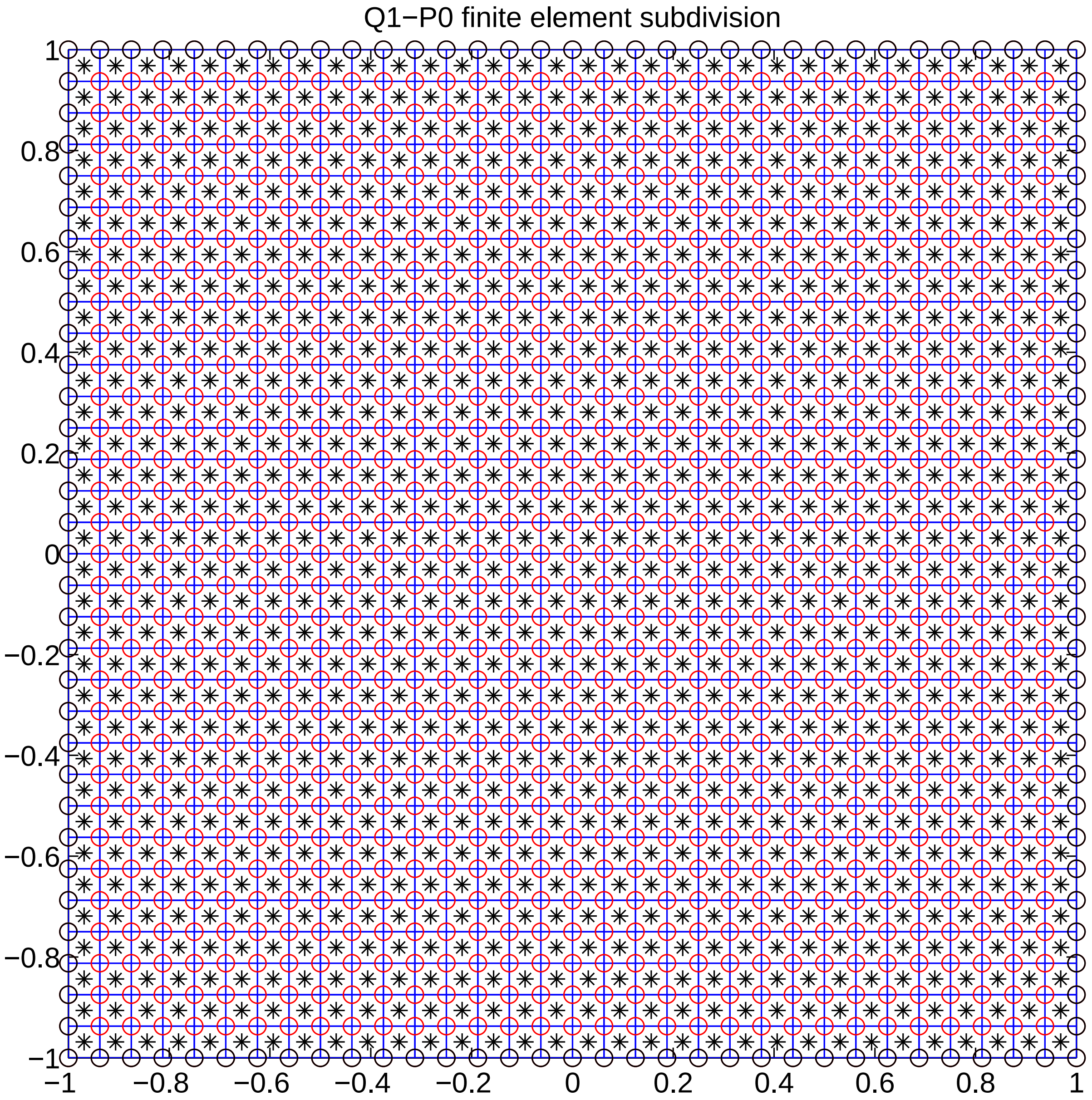
  lid-driven cavity

- square cavity $[-1,1] \times [-1,1]$
- flow induced by lid moving from left to right
- Dirichlet no-flow boundary condition on side and bottom boundaries
- different choices of nonzero horizontal velocity on the lid give rise to different computational models

$$\{y = 1; -1 \leq x \leq 1 | \quad u_x = 1 - x^4\}$$

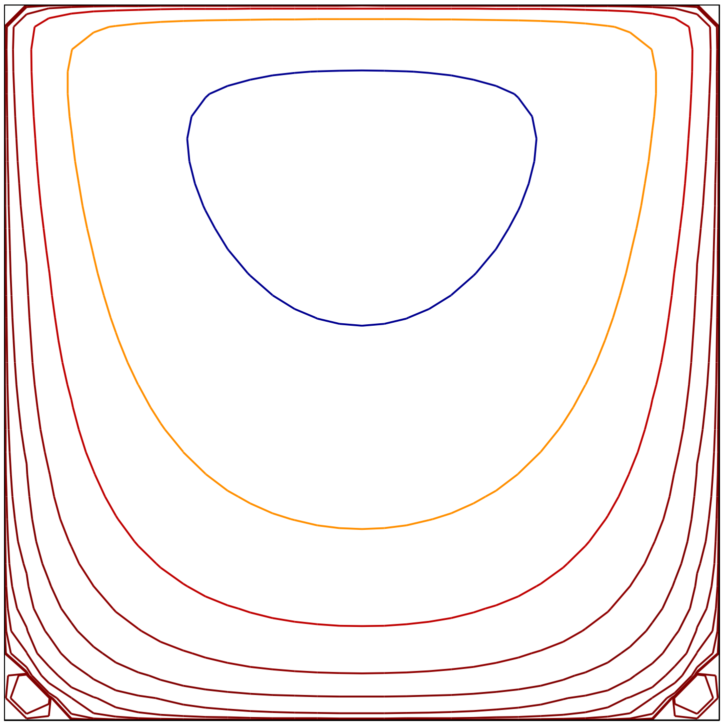
regularised cavity

Q1-P0 Discretisation

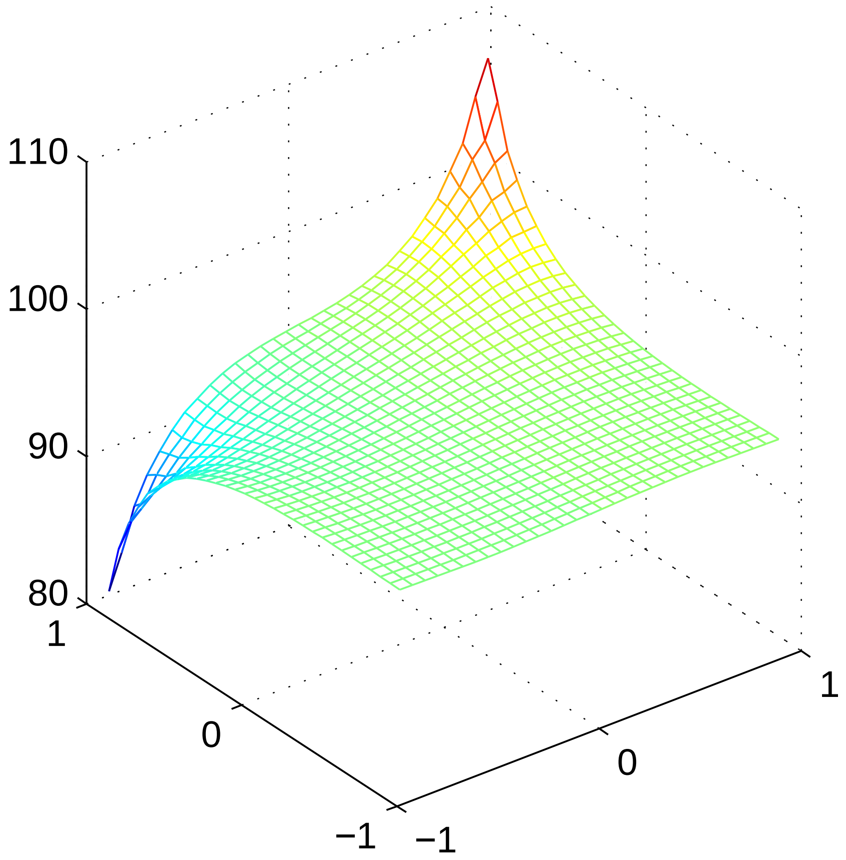


Typical Solution

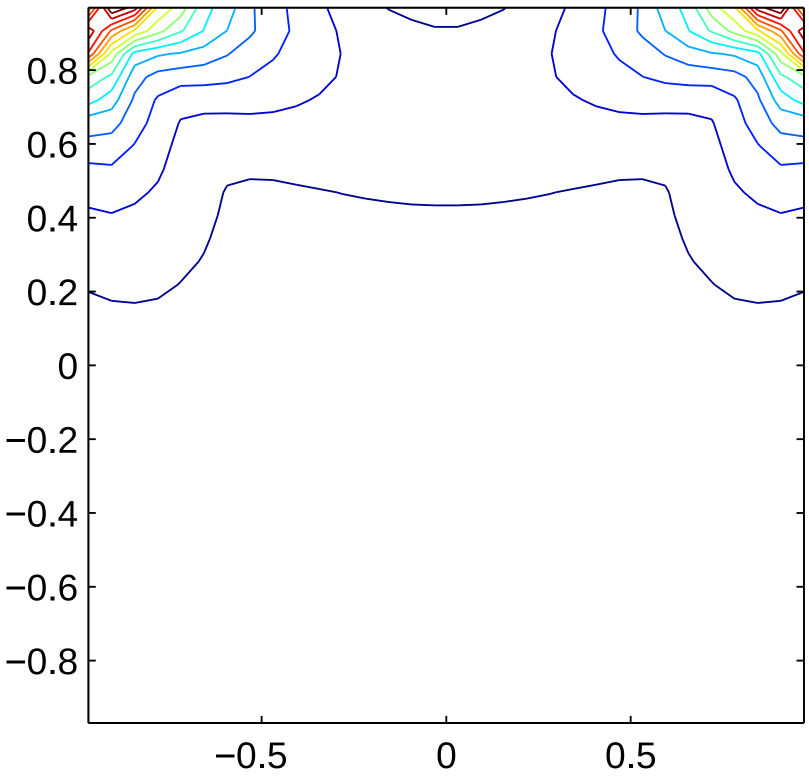
Streamlines: selected

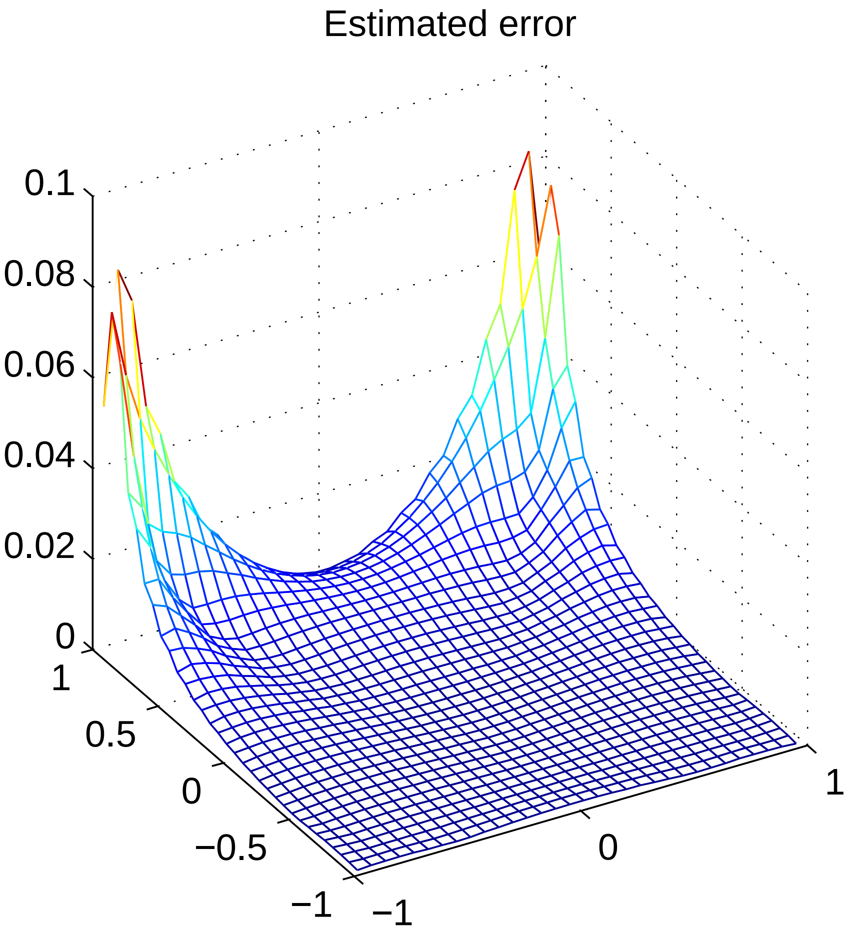


pressure field

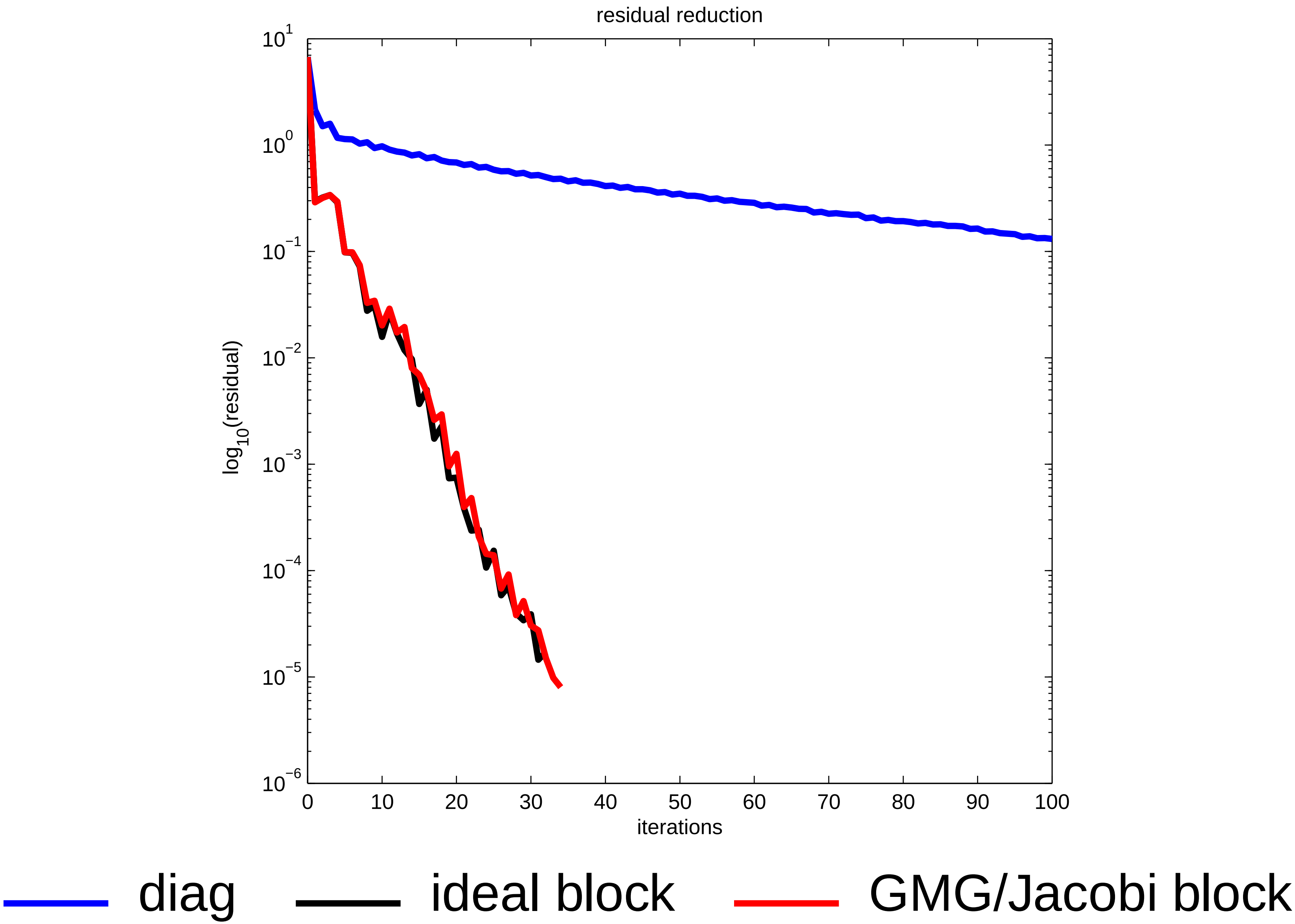


Estimated Error



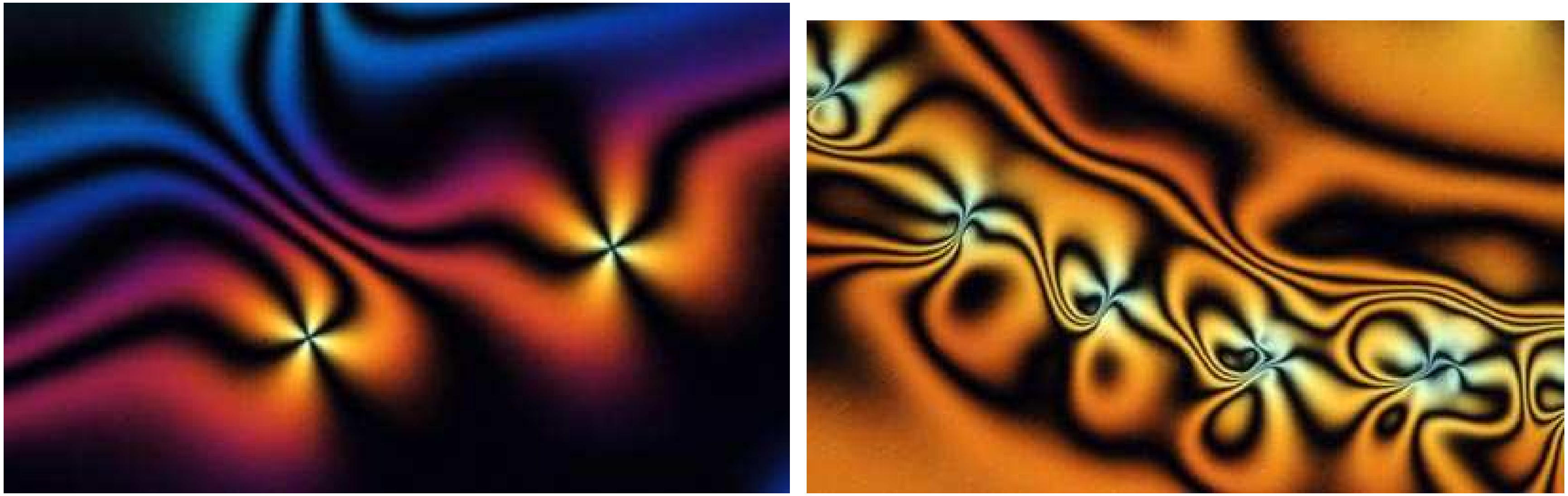


Sample Results: Stokes



Example 3: Liquid Crystal Modelling

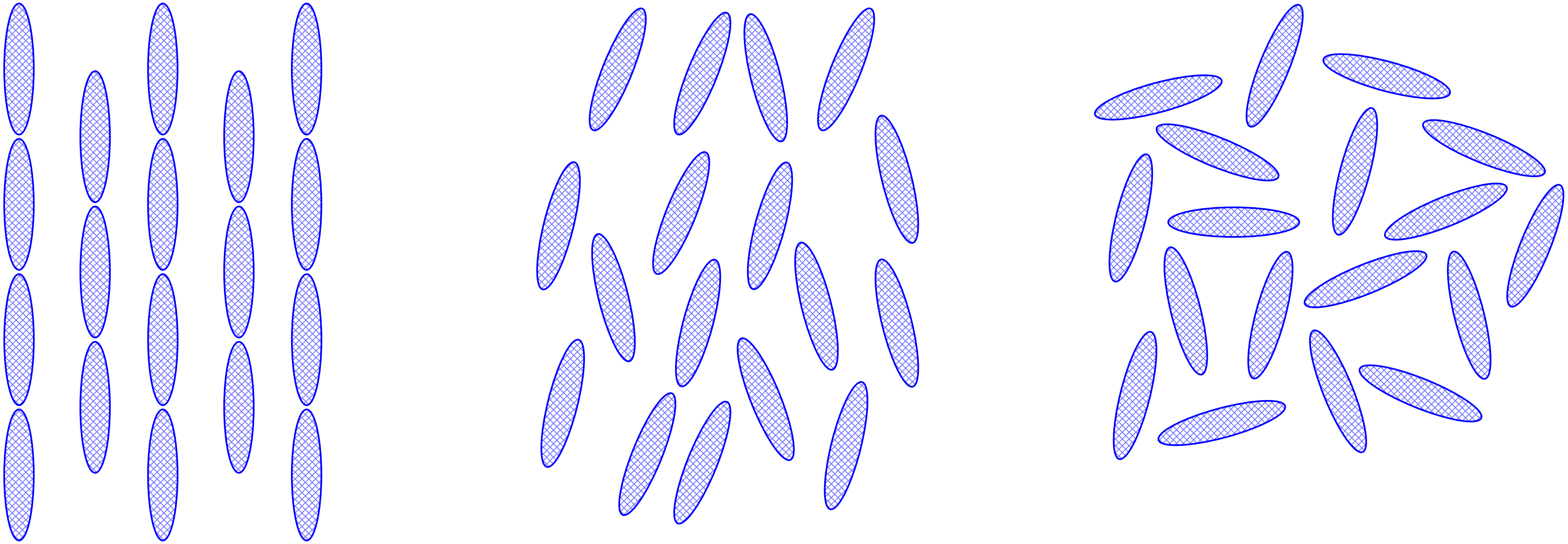
- LCDs ubiquitous in every-day life.
- More and more applications in e-readers, moving colour displays, digital ink. . .
- Require numerical models linking molecular orientation and flow.
- Joint work with André Sonnet (Strathclyde).



Photographs by Israel Lazo, Kent State University.

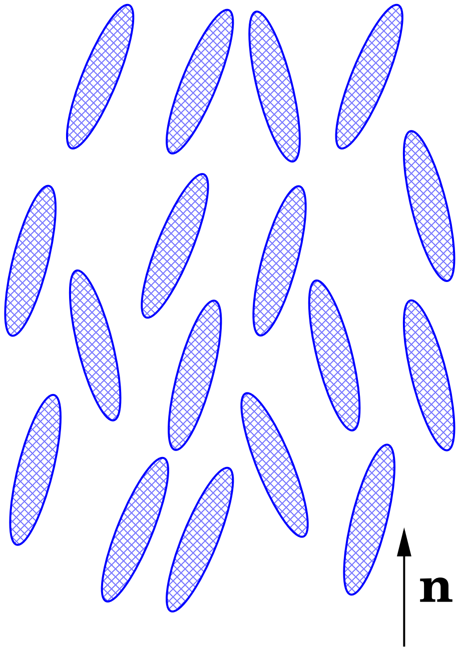
Liquid Crystals

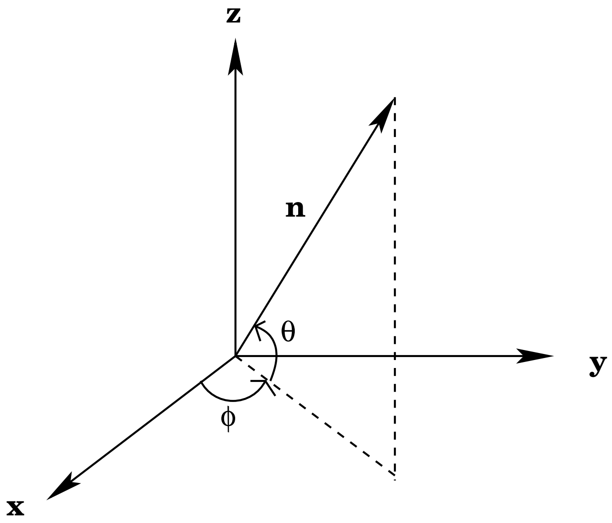
- occur between solid crystal and isotropic liquid states



- may have different equilibrium configurations
- switch between stable states by altering applied voltage, boundary conditions, . . .

Director Model





- director: average direction of molecular alignment

$$\mathbf{n} = (\cos\theta\cos\phi, \cos\theta\sin\phi, \sin\theta)$$

- order parameter: measure of orientational order

$$S = \frac{1}{2} < 3\cos^2\theta_m - 1 >$$

$\mathcal{Q}$-tensor Model

- tensor order parameter (symmetric and traceless)

$$\mathbf{Q} := \langle \overbracket{\boldsymbol{n} \otimes \boldsymbol{n}} \rangle = \langle \boldsymbol{n} \otimes \boldsymbol{n} - \frac{1}{3}\mathbf{I} \rangle$$

- material and co-rotational time derivatives

$$\dot{\mathbf{Q}} = \frac{\partial \mathbf{Q}}{\partial t} + (\nabla \mathbf{Q})\boldsymbol{v}, \qquad \mathring{\mathbf{Q}} = \dot{\mathbf{Q}} - 2\,\overbracket{\mathbf{W}\mathbf{Q}}$$

- flow with velocity $\boldsymbol{v}$

- symmetric and skew parts of the velocity gradient

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

Governing Equations

- dissipation $R = R(\overset{\circ}{\mathbf{Q}}, \mathbf{Q}, \mathbf{D})$
- stress tensor

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

- coupled equations for alignment and flow:

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

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

Sonnet and Virga Dissipative Ordered Fluids: Theories for Liquid Crystals, Springer 2012

Special Case

- free energy based on Landau-deGennes potential

$$\phi = \frac{1}{2}A(T)\,\mathrm{tr}\,\mathbf{Q}^2 - \frac{\sqrt{6}}{3}B\,\mathrm{tr}\,\mathbf{Q}^3 + \frac{1}{4}C(\mathrm{tr}\,\mathbf{Q}^2)^2$$

- coupled equations

$$\begin{aligned} \mathring{\mathbf{Q}} = \Delta\mathbf{Q} &\; - \; \partial\phi/\partial\mathbf{Q} - \mathrm{Tu}\,\mathbf{D} \\ \nabla p &\; - \; \Delta\boldsymbol{v} = \mathrm{div}\,\mathbf{F} \end{aligned}$$

$$\mathbf{F} = \mathrm{Bf}\left\{\tfrac{1}{\mathrm{Tu}}\left[\mathbf{Q}(\Delta\mathbf{Q}) - (\Delta\mathbf{Q})\mathbf{Q} - \nabla\mathbf{Q}\odot\nabla\mathbf{Q}\right] + \Delta\mathbf{Q} - \partial\phi/\partial\mathbf{Q}\right\}$$

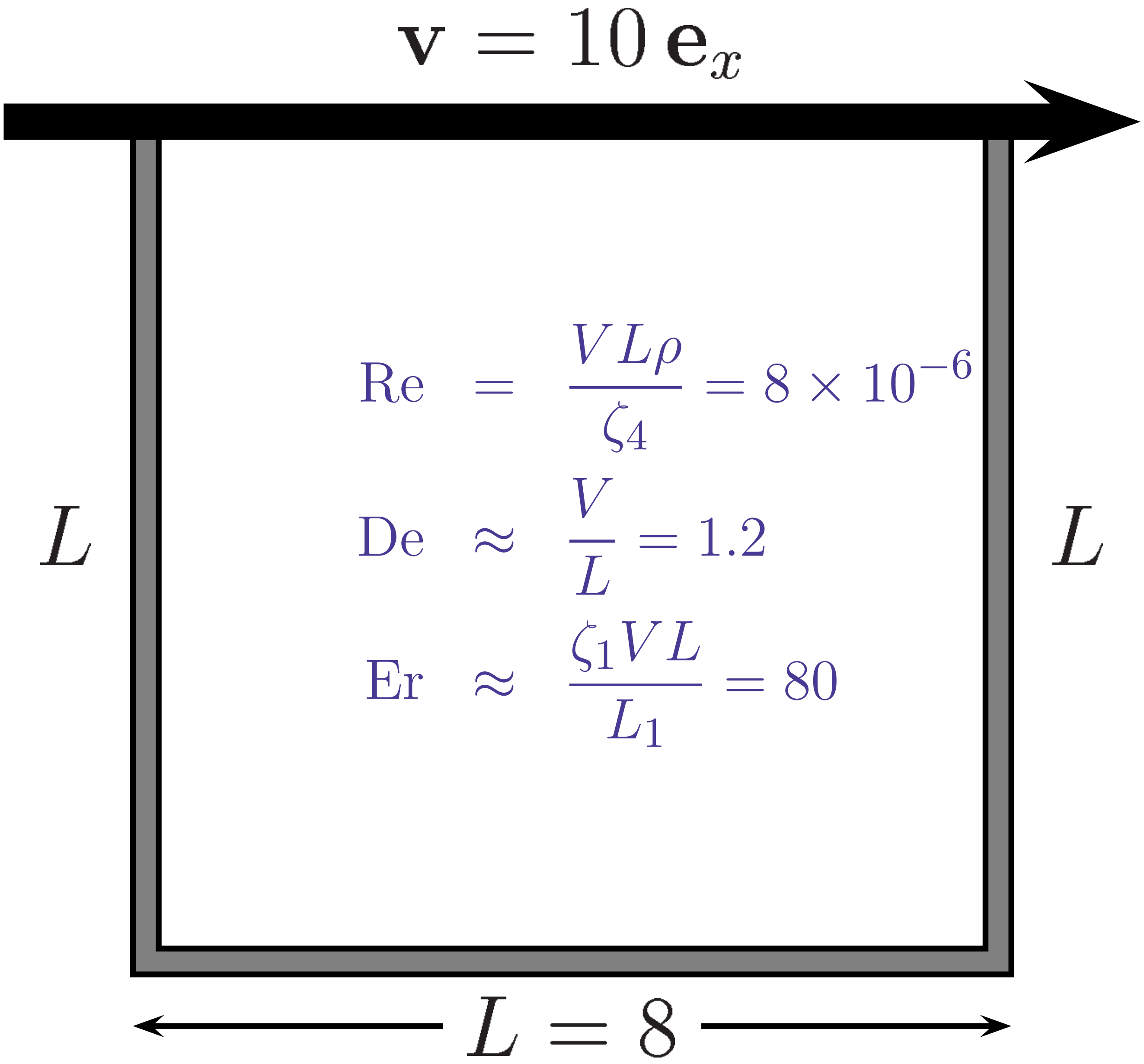
- the backflow parameter Bf measures the impact of the orientation on the flow;
- the tumbling parameter Tu measures the relative strength of problem viscosities.

Iterative Solution Strategy

- Decoupled solver:
  - For a given orientation field $\mathbf{Q}$, solve Stokes equation with $\boldsymbol{f} = \operatorname{div} \mathbf{F}$ as a body force.
  - Use the obtained flow field to compute one time step in a discretised version of the orientation equation.
  - Repeat with the new orientation field.

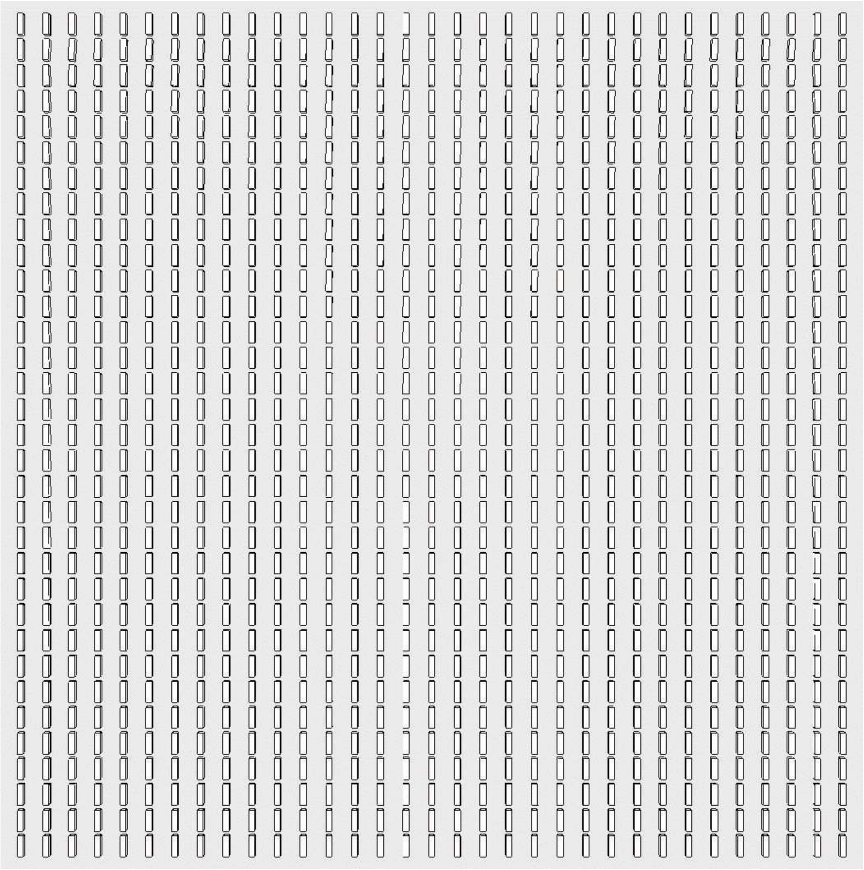
- Solution strategy
  - Orientation equation: finite difference scheme with explicit Euler time discretisation
  - Stokes equation: IFISS Stokes solver with multigrid preconditioning

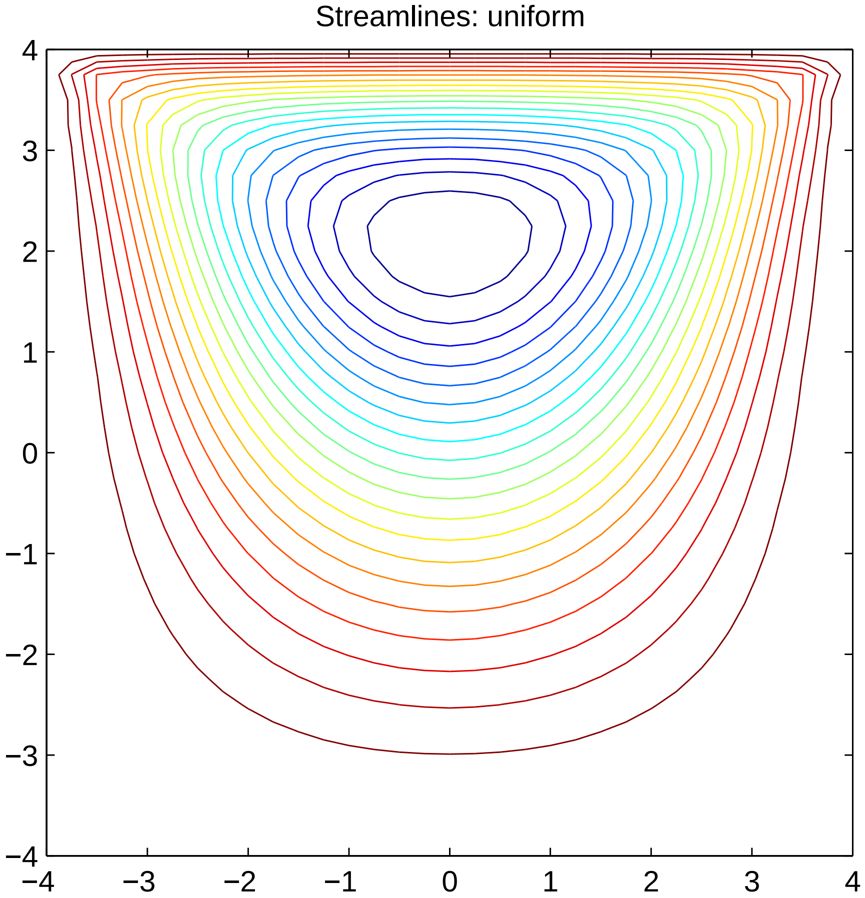
Lid Driven Cavity



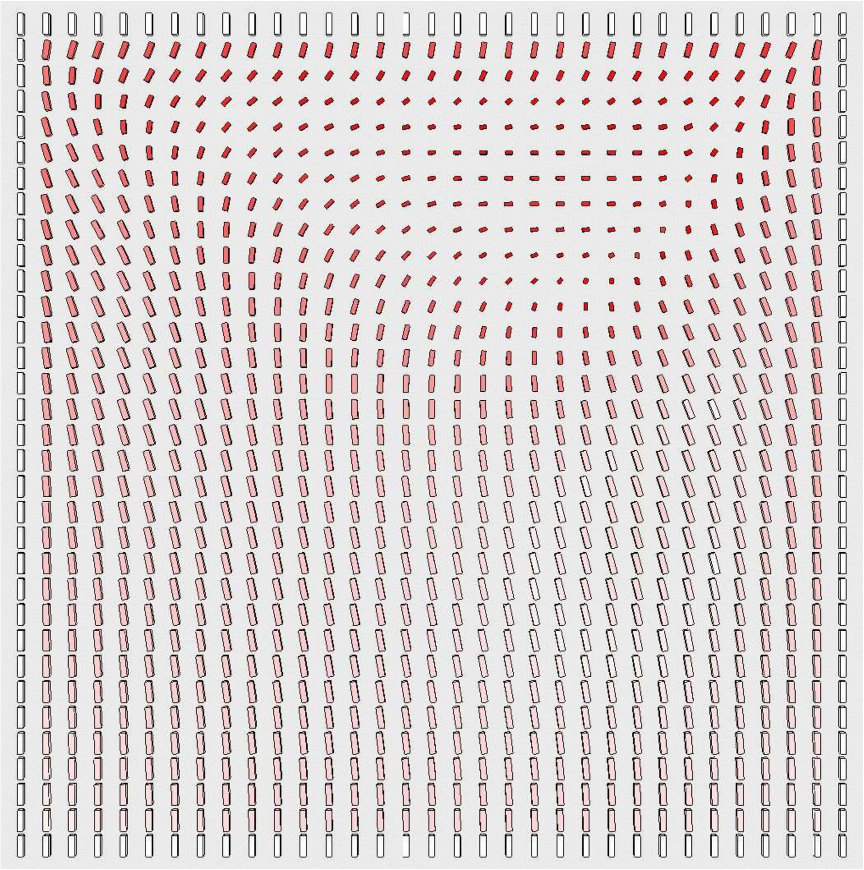
$$\begin{aligned} \mathrm{Re} &= \frac{VL\rho}{\zeta_4} = 8 \times 10^{-6} \\ \mathrm{De} &\approx \frac{V}{L} = 1.2 \\ \mathrm{Er} &\approx \frac{\zeta_1 V L}{L_1} = 80 \end{aligned}$$

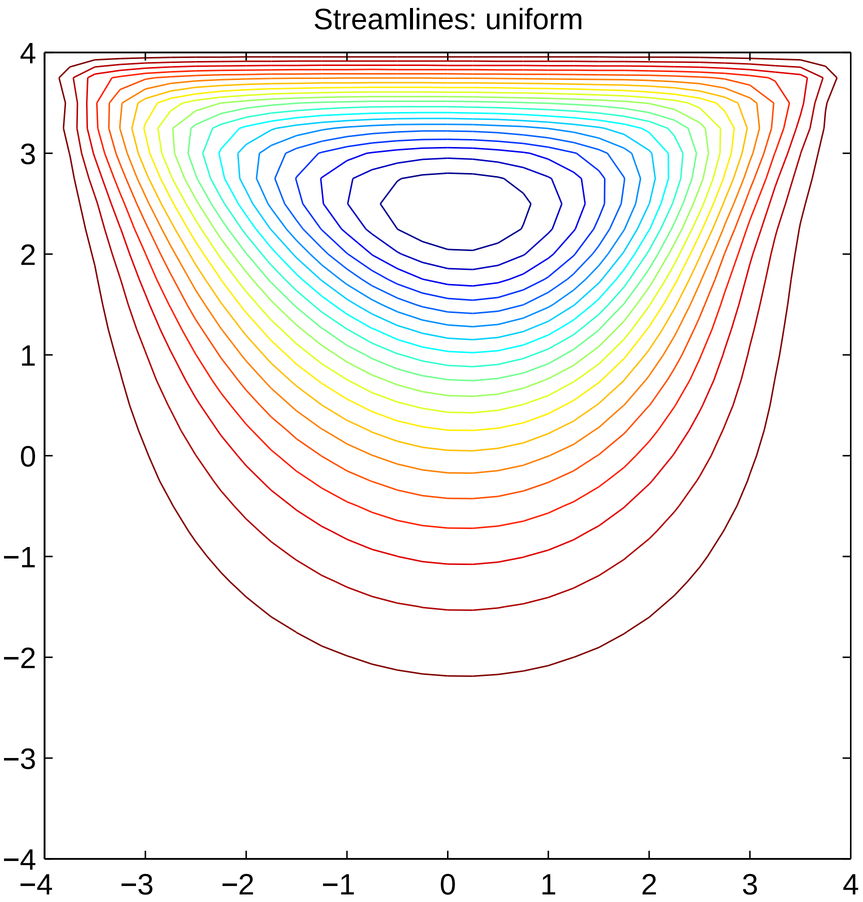
Initial Orientation and Flow Field



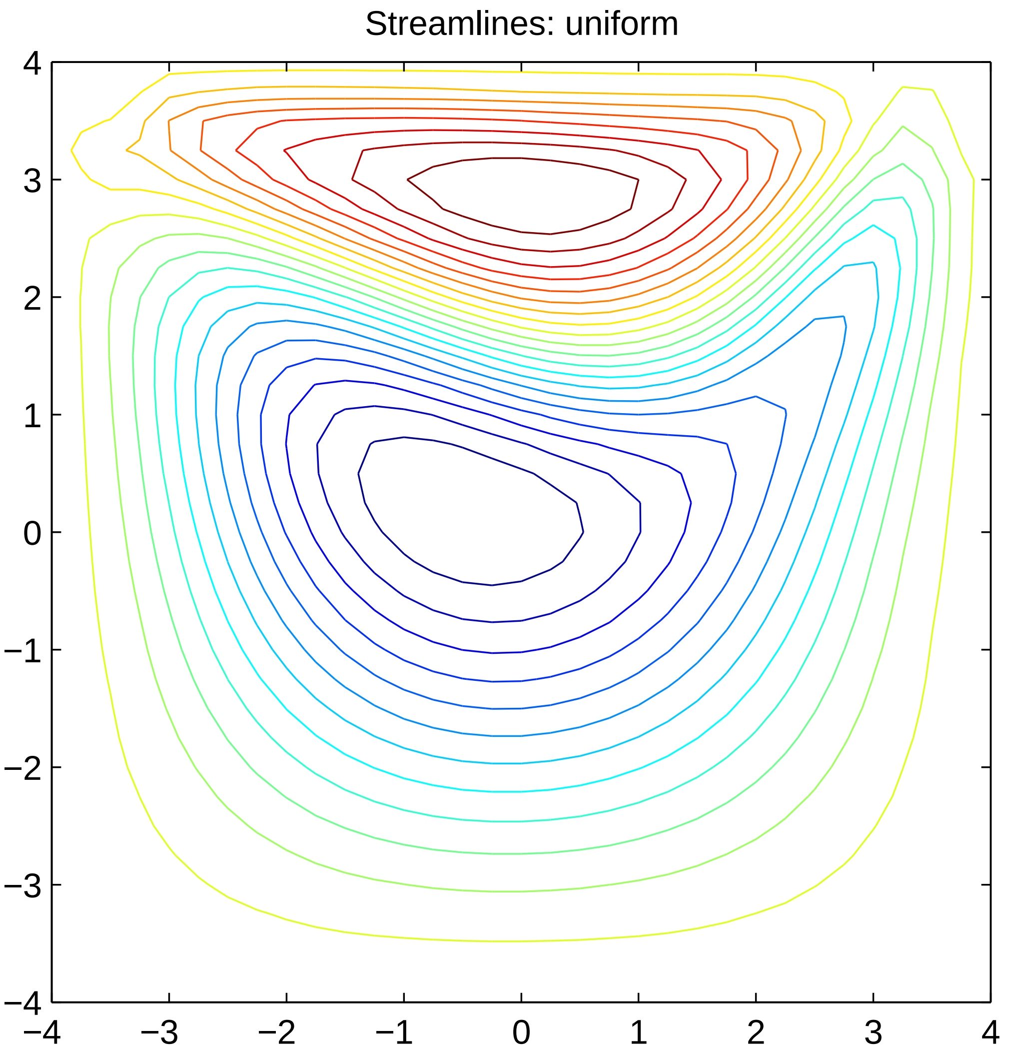


Later Orientation and Flow Field

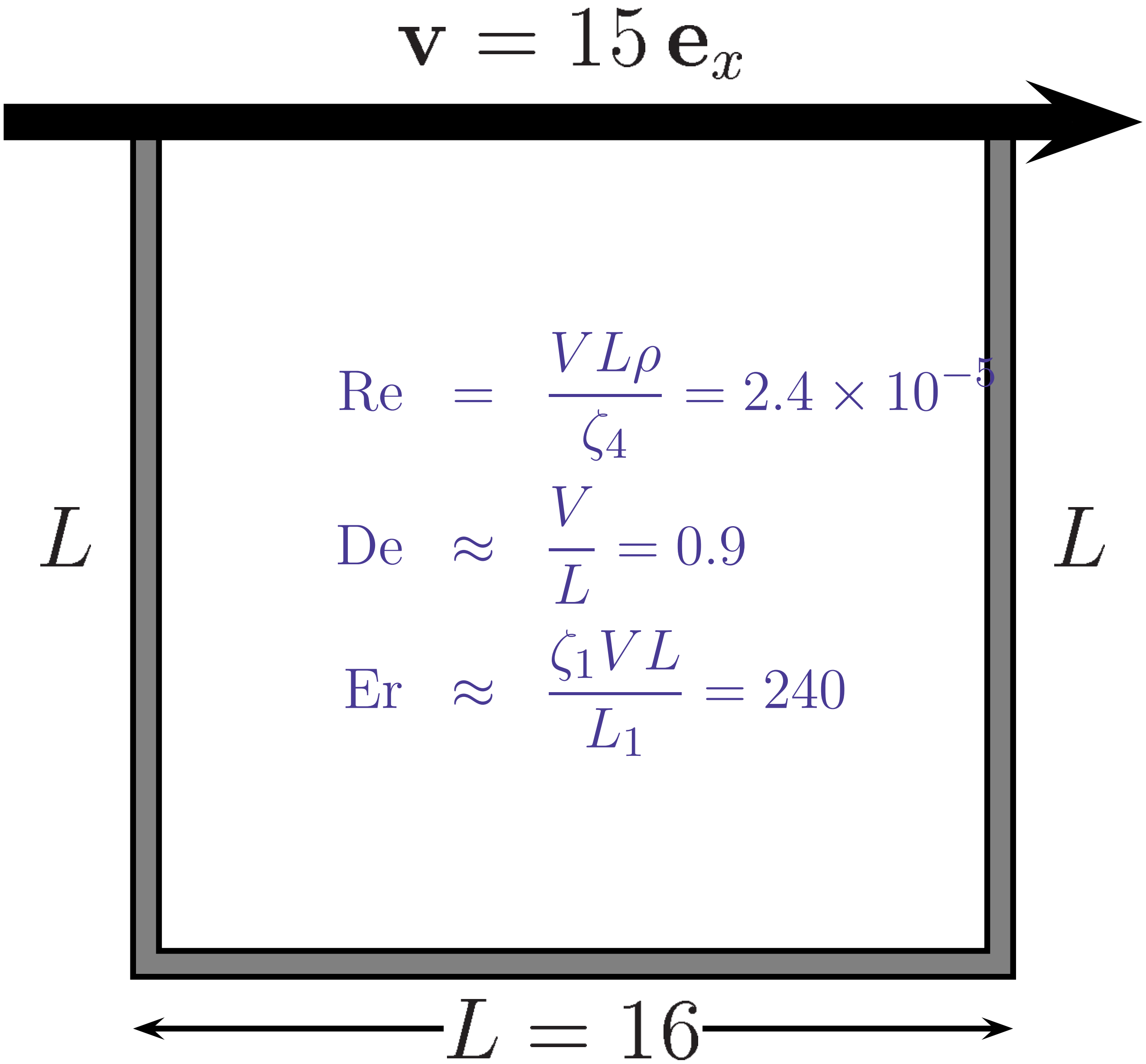




Flow Field Difference

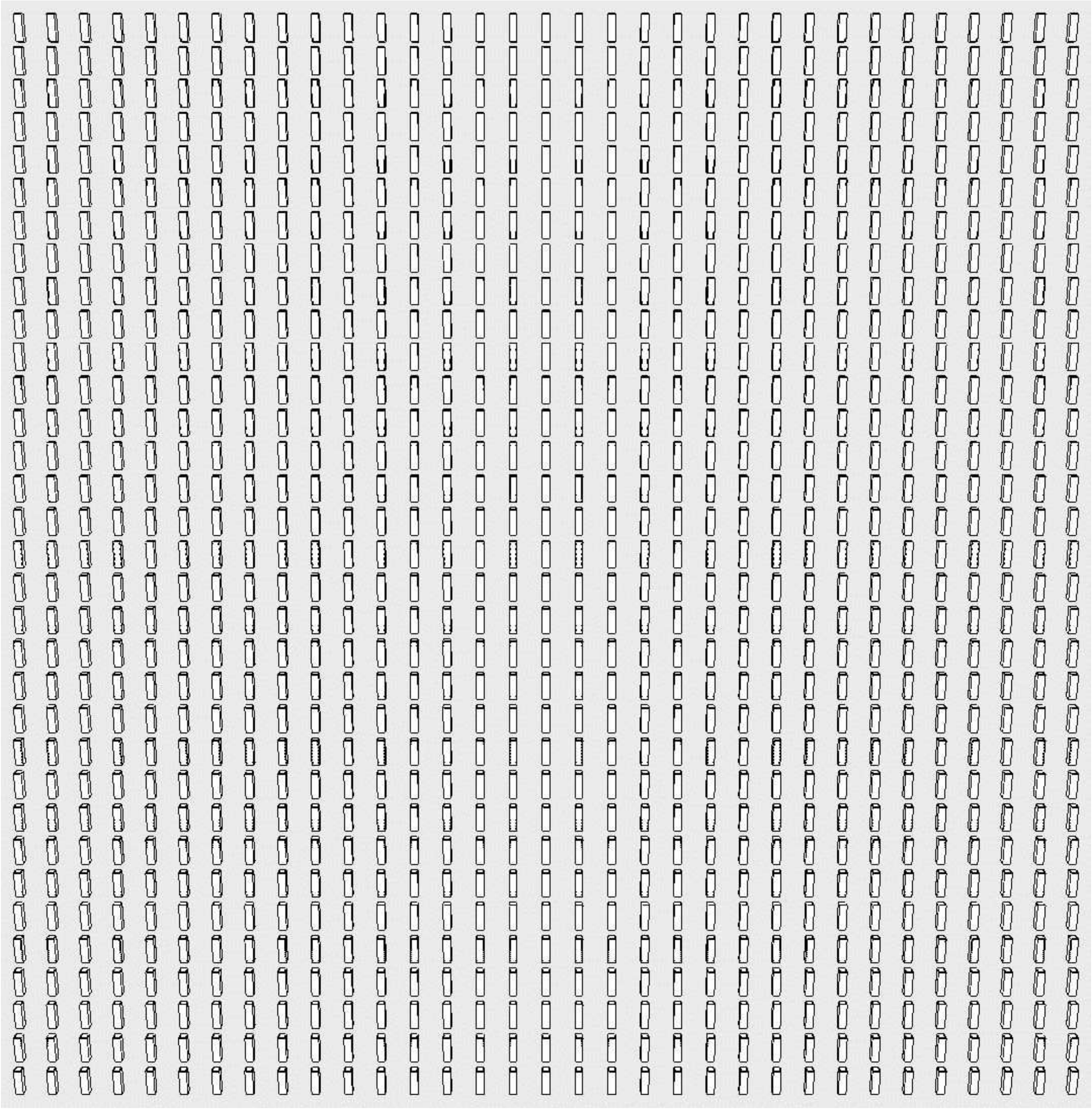


Out of Plane Orientation

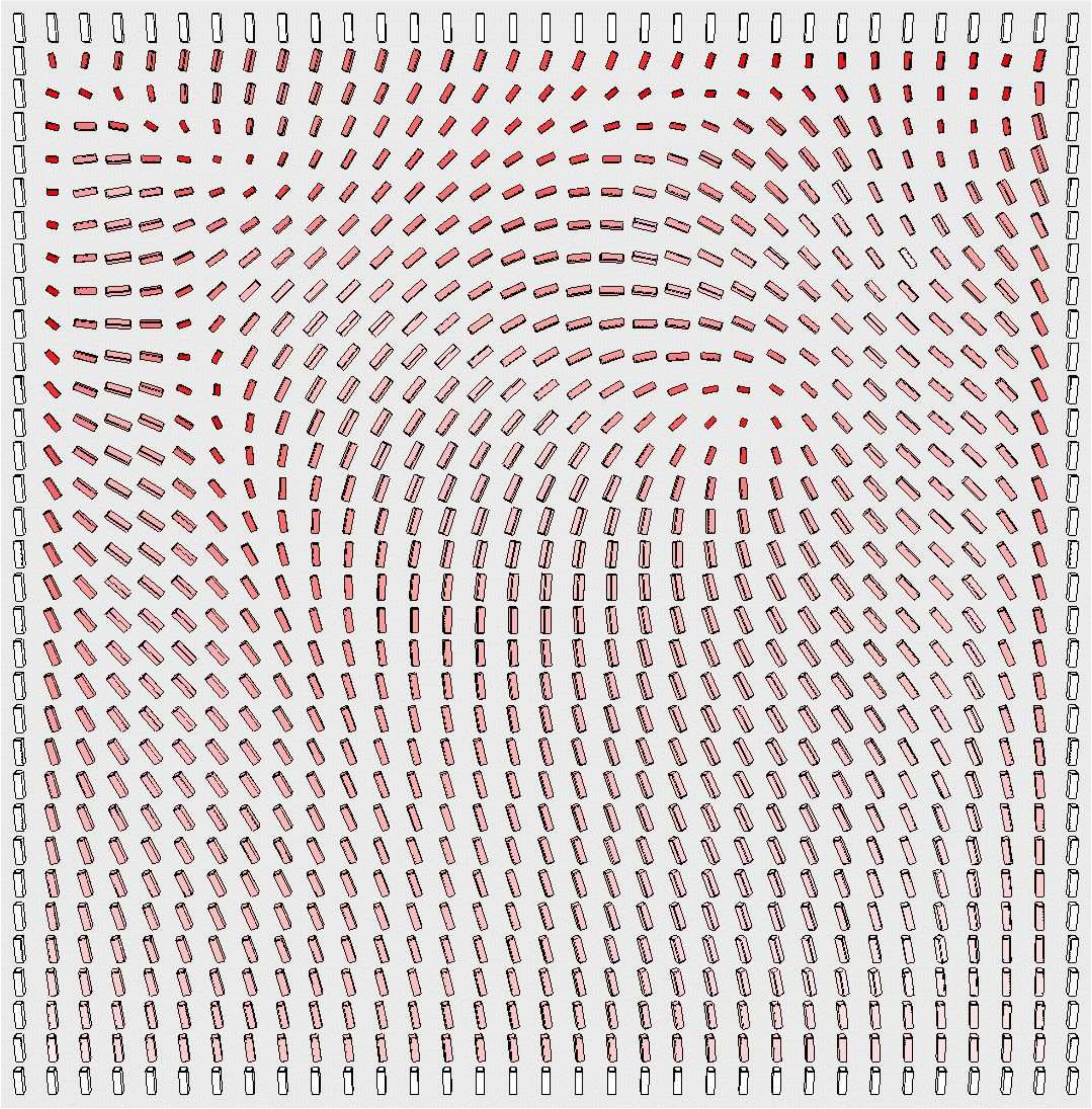


$$\begin{aligned}\mathrm{Re} &= \frac{VL\rho}{\zeta_4} = 2.4 \times 10^{-5}\\ \mathrm{De} &\approx \frac{V}{L} = 0.9\\ \mathrm{Er} &\approx \frac{\zeta_1 VL}{L_1} = 240\end{aligned}$$

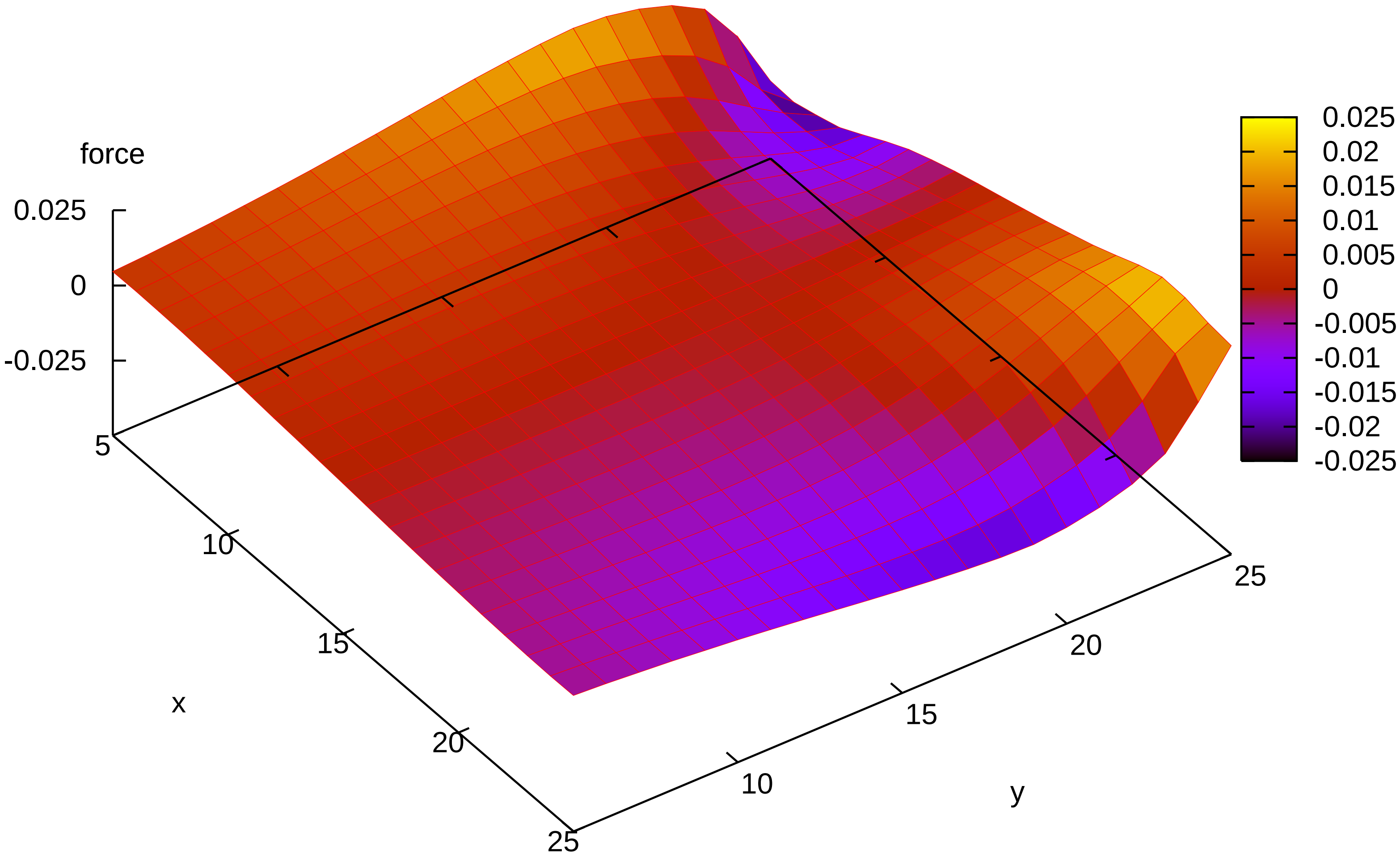
Initial Orientation



Later Orientation

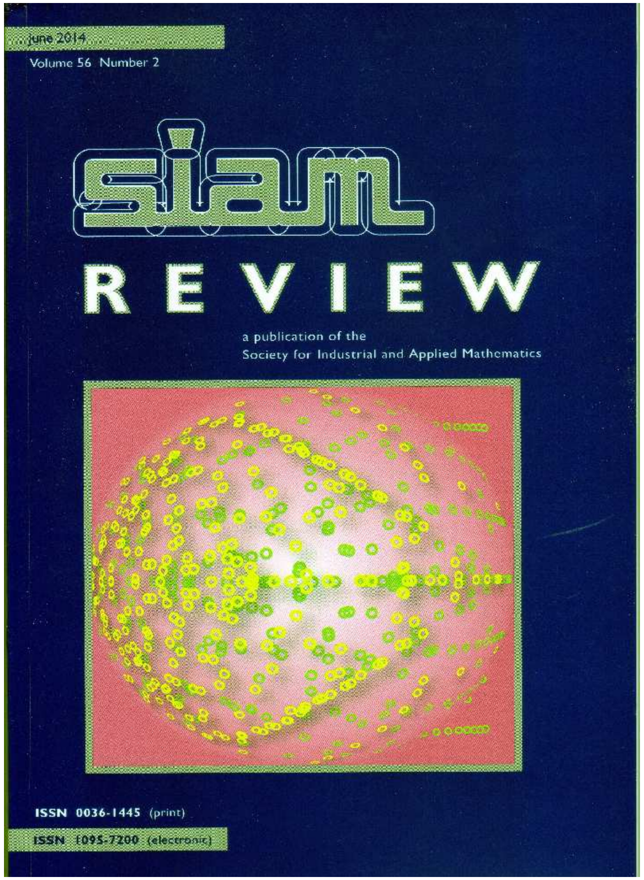


Out of Plane Force



Summary

- IFISS is a useful tool in teaching and research.
    - Useful source of benchmark problems.
    - Provides a convenient starting point for new problem classes, discretisations or solution algorithms.
    - Allows the study of both discretisation and iterative solution algorithms.
    - Easy to examine the interaction between the two and hence the resulting effect on overall solution cost.
- P-IFISS package for solving potential flow problems (Silvester and Powell 2007).
- New S-IFISS package for solving stochastic diffusion problems (Silvester, Bespalov and Powell 2014).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`www.cs.umd.edu/~elman/ifiss`

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