# Efficient solution techniques for the incompressible Stokes problem

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# Outline

# Culgi

- international company
- 10+ employees
- participation in EU projects
- simulation software for chemical processes
- support

# Scales of molecular modelling

- single atoms
- single molecule or cluster of molecules
- continuum

# Dynamic density field theory

- mixture of molecules of different types
- continuum hypothesis: density of molecules (per type)
- evolution equation: dynamics of molecules
- velocity obtained via the Stokes equations

# Cartesian tensor notation & Einstein notation

- element of vector is denoted by subscript:

$$\vec{\phi} = [\phi_1, \phi_2, \phi_3]$$

- differentiation is denoted as

$$\phi_{,\alpha} = \frac{d\phi}{dx_\alpha}$$

- Einstein summation convention:

$$\phi_{\alpha,\alpha} = \phi_{1,1} + \phi_{2,2} + \phi_{3,3}$$

# The Navier-Stokes equations

- conservation of mass:

$$\rho_{,t} + (\rho u_\alpha)_{,\alpha} = 0$$

- conservation of mass for incompressible flow:

$$u_{\alpha,\alpha} = 0$$

- conservation of momentum for incompressible flow:

$$\rho u_{\alpha,t} + \rho u_{\alpha,\beta} u_\beta = -p,\alpha + \nu(u_{\alpha,\beta} + u_{\beta,\alpha})_{,\beta} + \rho f_\alpha^b$$

# The Stokes equations

- viscous flow, neglect inertia term in momentum equation:

$$(\nu(u_{\alpha,\beta} + u_{\beta,\alpha}))_{,\beta} - p_{,\alpha} = -\rho f_{\alpha}^{b}$$

- body force $\vec{f}^{b}$ acts on molecules of the same type:

$$\rho\vec{f}^{b} = \rho_i \vec{f}_i^{b}$$

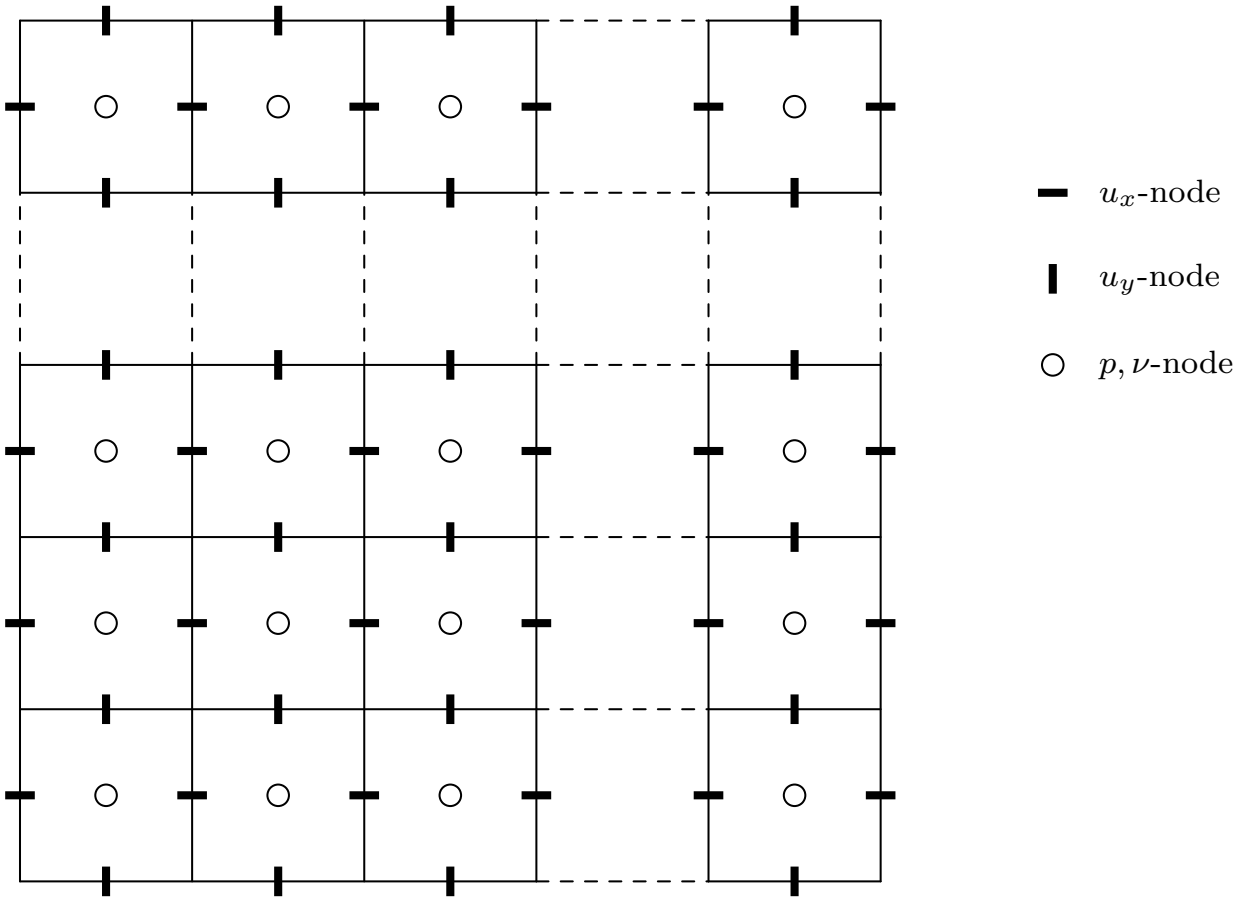
- viscosity is a weighted average of the molecule viscosities:

$$\nu = \nu_i \rho_i$$

# Discretisation

- staggered grid
- finite difference

# Staggered grid

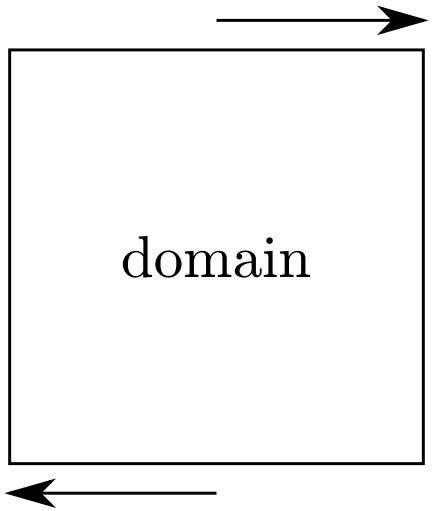


# Domain

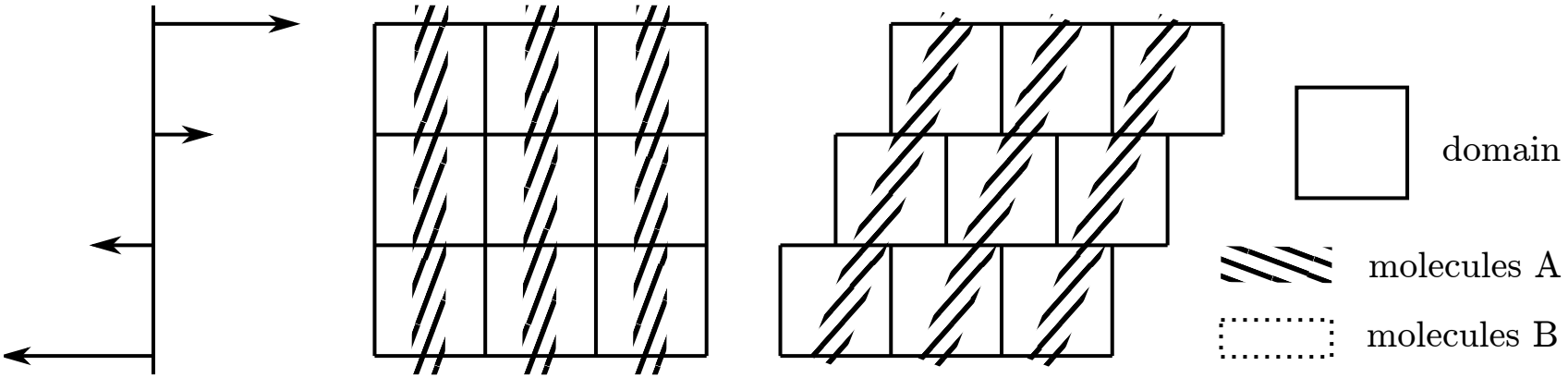
- grid size is comparable to the size of the molecules
- physical dimensions of simulated domain is small
- periodic boundaries

# Shear velocity

- modelling stirring or flow near solid wall
- velocity difference between two sides of the domain



# Shifting boundaries




velocity profile $t=0$ $t>0$

# Saddle point system

- Stokes equations:

$$\begin{bmatrix} F & B^T \\ B & O \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix}$$

- $F$: $n \times n$ Laplace operator, symmetric positive semidefinite
- $B^T$: $n \times m$ gradient operator
- $B$: $m \times n$ divergence operator
- complete system is symmetric
- ill-conditioned

# Singular system

- system is singular due to periodic boundary conditions
- replace system by one with equivalent solution
- augmented Lagrangian:

$$\begin{bmatrix} F + B^T W B & B^T \\ B & O \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix}$$

# Schur complement

- block Cholesky decomposition:

$$\begin{bmatrix} F & B^T \\ B & O \end{bmatrix} = \begin{bmatrix} I & O \\ BF^{-1} & I \end{bmatrix} \begin{bmatrix} F & O \\ O & S \end{bmatrix} \begin{bmatrix} I & F^{-1}B^T \\ O & I \end{bmatrix}$$

- Schur complement: $S = -BF^{-1}B^T$
- dense $m \times m$ matrix

# Schur complement reduction

$$\begin{bmatrix} F & B^T \\ O & S \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} f \\ -BF^{-1}f \end{bmatrix}$$

- (block) direct method
- accuracy of subsystems
- iterative extension

# Null space method

- $Z$: null space of divergence operator $B$
- $u \in \text{col}(Z)$: let $u = Zv$
- $Z^T F Z v + Z^T B^T p = Z^T F Z v = Z^T f$
- basis of the null space
- Fourier modes
- $F$-orthogonal: $Z^T F Z = I$

# Block triangular preconditioner

$$P = \begin{bmatrix} \tilde{F} & B^T \\ O & \tilde{S} \end{bmatrix}$$

- $\tilde{F} \approx F$ and $\tilde{S} \approx S$
- exact solution in two iterations when $F$ and $S$ exact
- triangular versus diagonal

# Approximating the Schur complement

- cheap inverse
- $S \approx -I$
- $S \approx -2I\nu^{-1}$
- approximate commutator

$$\mathcal{F}\mathcal{G} = \mathcal{G}\mathcal{F}_p$$

$$\mathcal{S} \approx -(\mathcal{G}^*\mathcal{G})\mathcal{F}_p^{-1}$$

# Deflation

- Krylov subspace augmented by a deflation subspace
- choice of deflation vectors
- works in conjunction with preconditioners

# Backend/library

- various simulation models
- vectors with discrete operators
- non-linear equation solver
- parallel computations using MPI and OpenMP
- no support for (sparse) matrices

# Frontend

- GUI
- TCL and Python

# The Stokes equations

- implicit matrix vector products using discrete operators

$$\mathcal{D}\left(\nu\left(\mathcal{G}u + \mathcal{G}^T\vec{u}\right)\right) - \mathcal{G}p = -\rho f^b$$

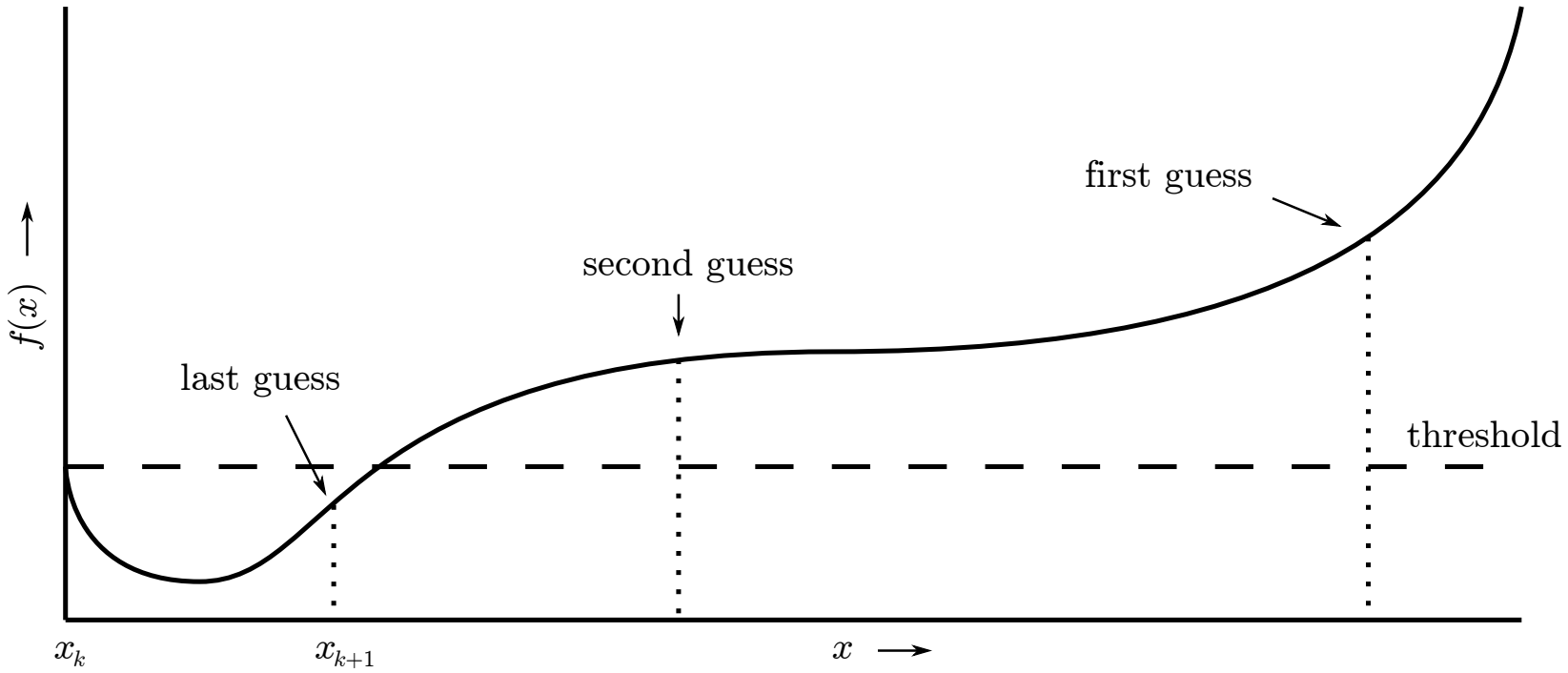
$$\mathcal{D}\vec{u} = 0$$

- boundary conditions:
  - extending grid
  - applying periodicity

# Steepest descent with line search

- start with initial guess $x_0$
- repeat until converged:
  - determine gradient $(r_k)$
  - find 'optimal' solution in direction of gradient starting from $x_k$

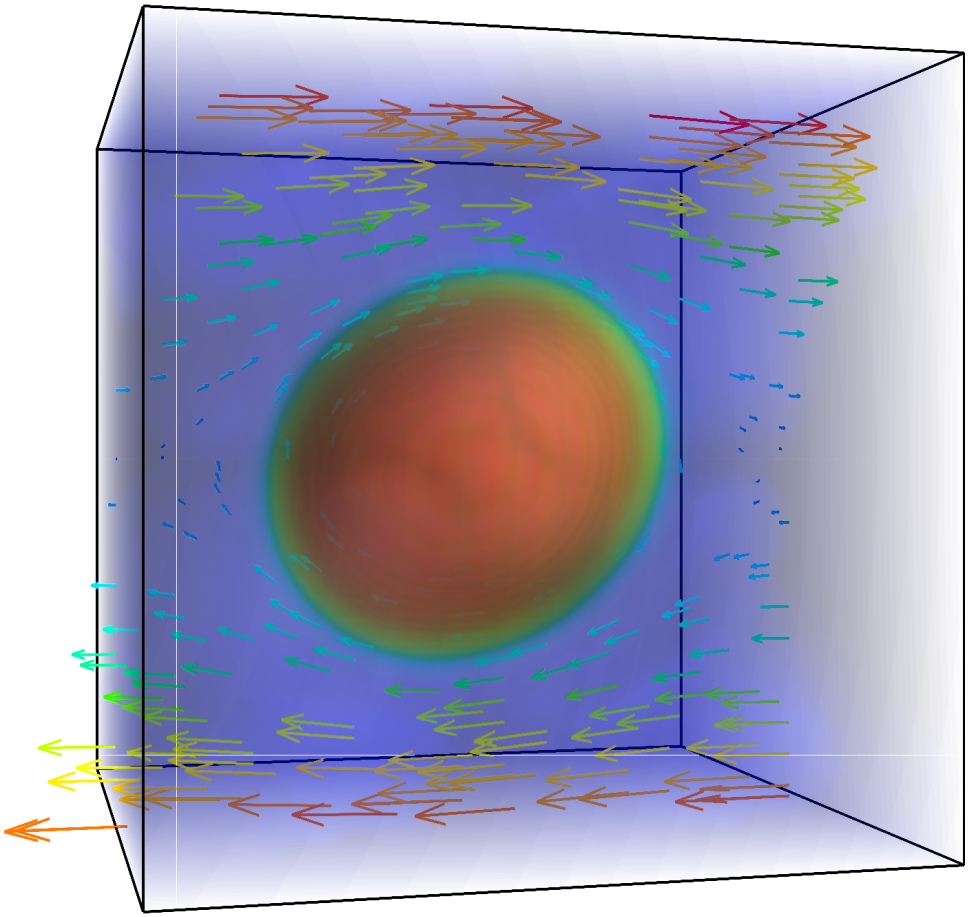
# Line search



# Oil droplet

- oil droplet suspend in water
- oil viscosity is higher than water viscosity
- sharpness of interface

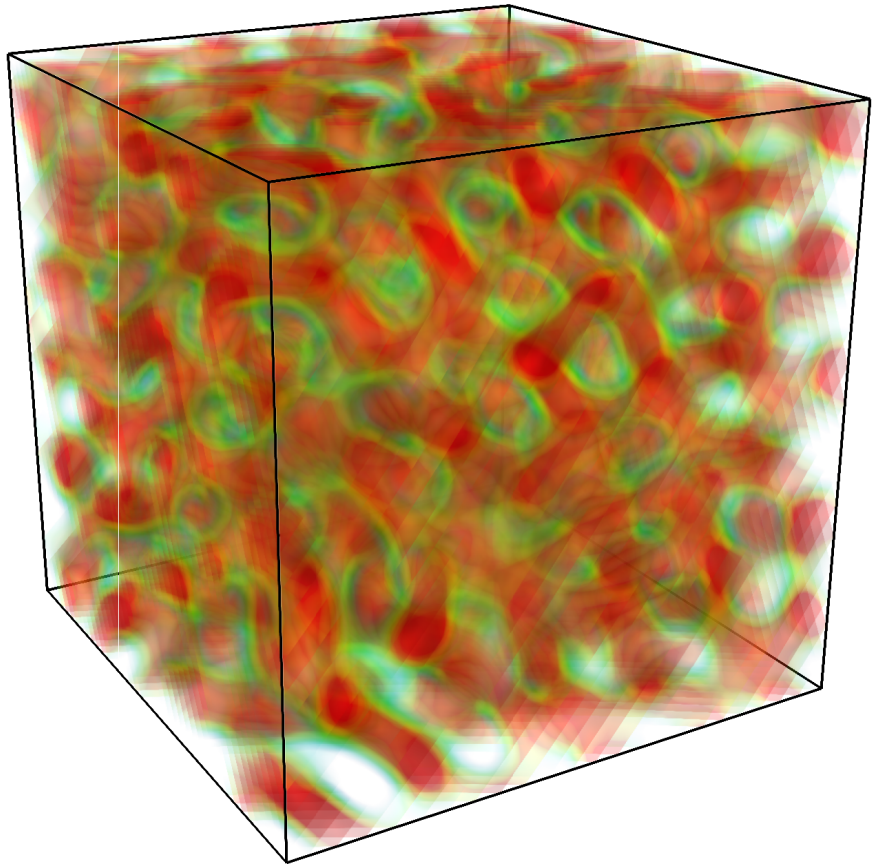
# Oil droplet



# Diblock copolymer blend

- reaction with molecules $\mathcal{A}$ and $\mathcal{B}$: polymers $\mathcal{AA}$, $\mathcal{AB}$ and $\mathcal{BB}$
- $\mathcal{A}$ and $\mathcal{B}$ repel each other
- typical polymer: $\mathcal{AAABAABABBBBABBB}$
- approximate polymer: $\mathcal{AAAAAAAABBBBBBBB}$
- chaotic initial state
- shearing creates laminar or cylindrical phases

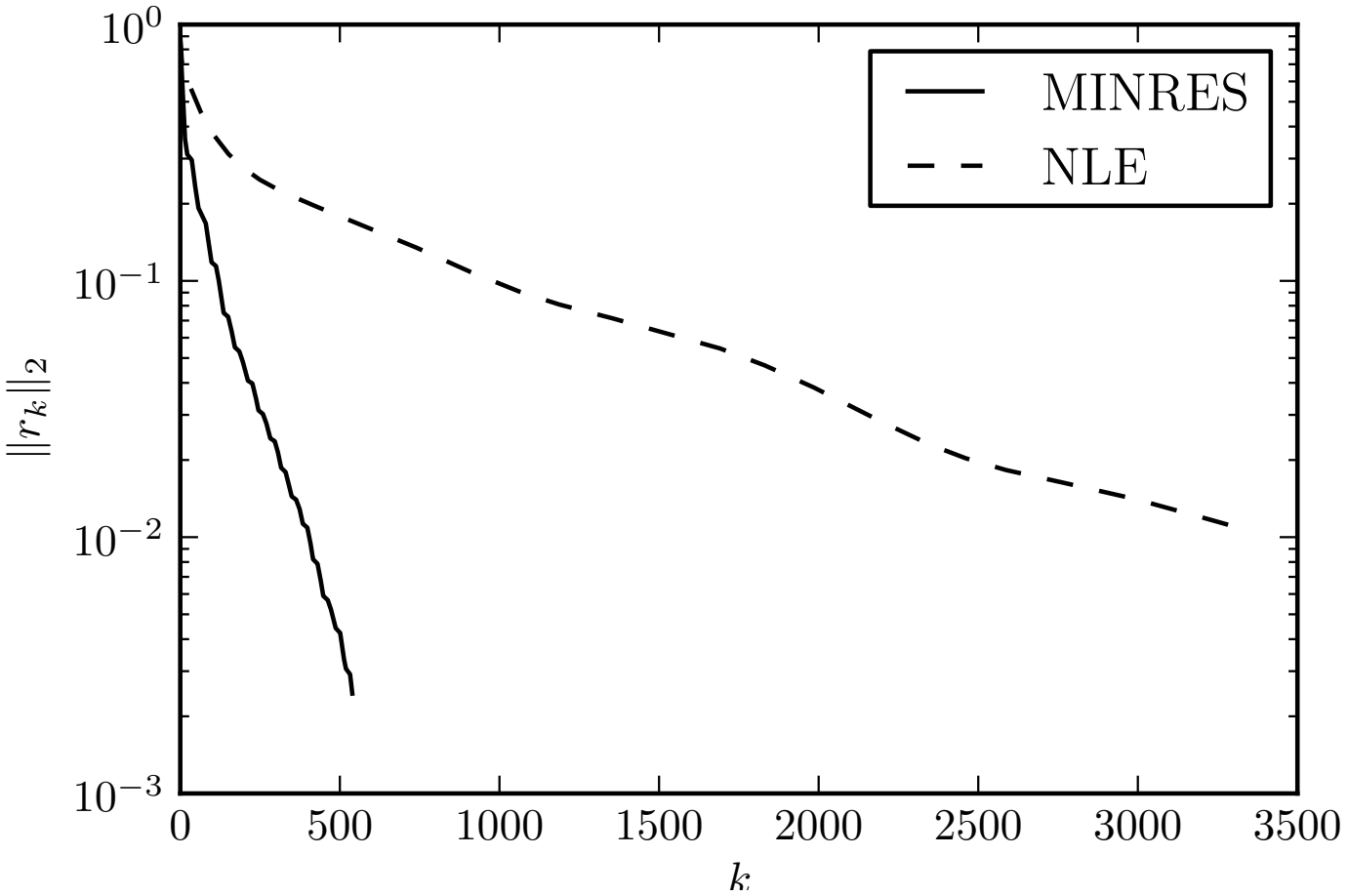
# Diblock copolymer blend



# Simulation

- oil droplet
- NLE versus MINRES

# Rate of convergence (grid: $64^3$, oil viscosity: 10)



# Rate of convergence for varying grid sizes

| box type | box size | NLE iter. | NLE l.s. tot. iter. | MINRES iter. |
|---|---|---|---|---|
| 2d | 16 | 346 | 695 | 63 |
| | 32 | 1176 | 2354 | 172 |
| | 64 | 2798 | 5598 | 359 |
| | 128 | 3446 | 6894 | 504 |
| 3d | 16 | 363 | 729 | 99 |
| | 32 | 1083 | 2169 | 269 |
| | 64 | 2293 | 4589 | 558 |
| | 128 | 4411 | 8825 | 770 |

# Rate of convergence for varying viscosity

| box type | oil viscosity | NLE iter. | NLE l.s. tot. iter. | MINRES iter. |
|---|---|---|---|---|
| 2d | 10.0 | 1176 | 2354 | 172 |
| | 20.0 | 2524 | 5051 | 248 |
| | 40.0 | 4986 | 9976 | 343 |
| | 100.0 | *did not converge* | | 498 |
| | 1000.0 | *did not converge* | | 1225 |
| 3d | 10.0 | 1083 | 2169 | 269 |
| | 20.0 | 2115 | 4234 | 472 |
| | 40.0 | 4505 | 9015 | 676 |
| | 100.0 | *did not converge* | | 1057 |
| | 1000.0 | *did not converge* | | 2974 |

- limited to ‘simple’ solution techniques
- block triangular preconditioner
- deflation
- null space method
- initial guess