MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

NUMERICAL LINEAR ALGEBRA
FOR DYNAMICAL SYSTEMS

Fast Iterative Solvers for a Coupled Cahn–Hilliard/Navier–Stokes System

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Christian Kahle
(Universität Hamburg).

1. Motivation

2. Diffuse Interface Approach

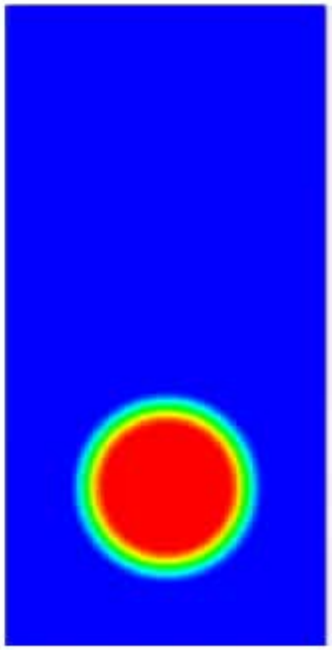
3. Cahn–Hilliard/Navier–Stokes Model

4. Linear Systems and Preconditioning

5. Numerical Results

Setting

- two-phase flow
- two immiscible, incompressible viscous fluids
- different physical properties
  - densities $\tilde{\rho}_1$, $\tilde{\rho}_2$
  - viscosities $\tilde{\eta}_1$, $\tilde{\eta}_2$
- diffuse interface model
  - to cope with topological changes

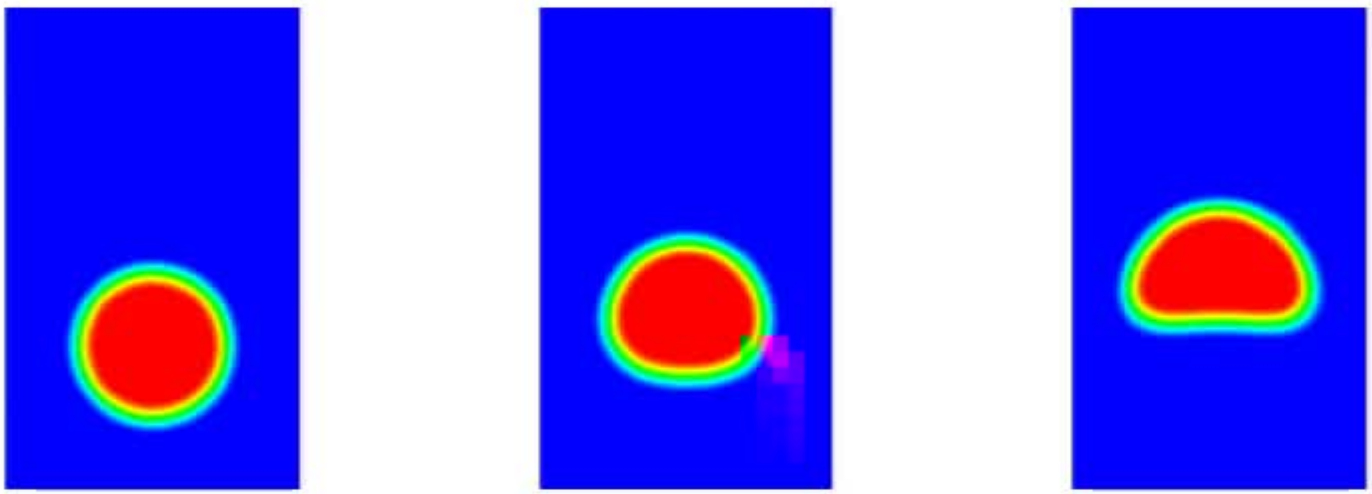


Motivation

Examples

Model for the dynamics of multiphase fluids

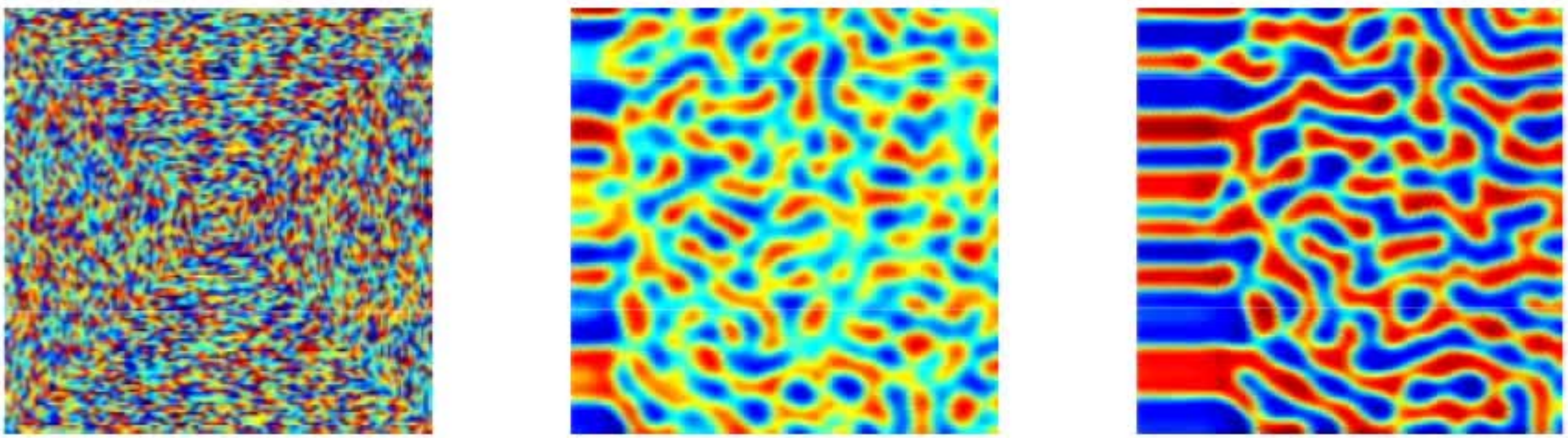
- rising bubble / falling droplet



Examples

Model for the dynamics of multiphase fluids

- rising bubble / falling droplet
- mixing of fluids in a driven cavity
- spinodal decomposition under shear



[Kay/Welford '07]

Examples

Model for the dynamics of multiphase fluids

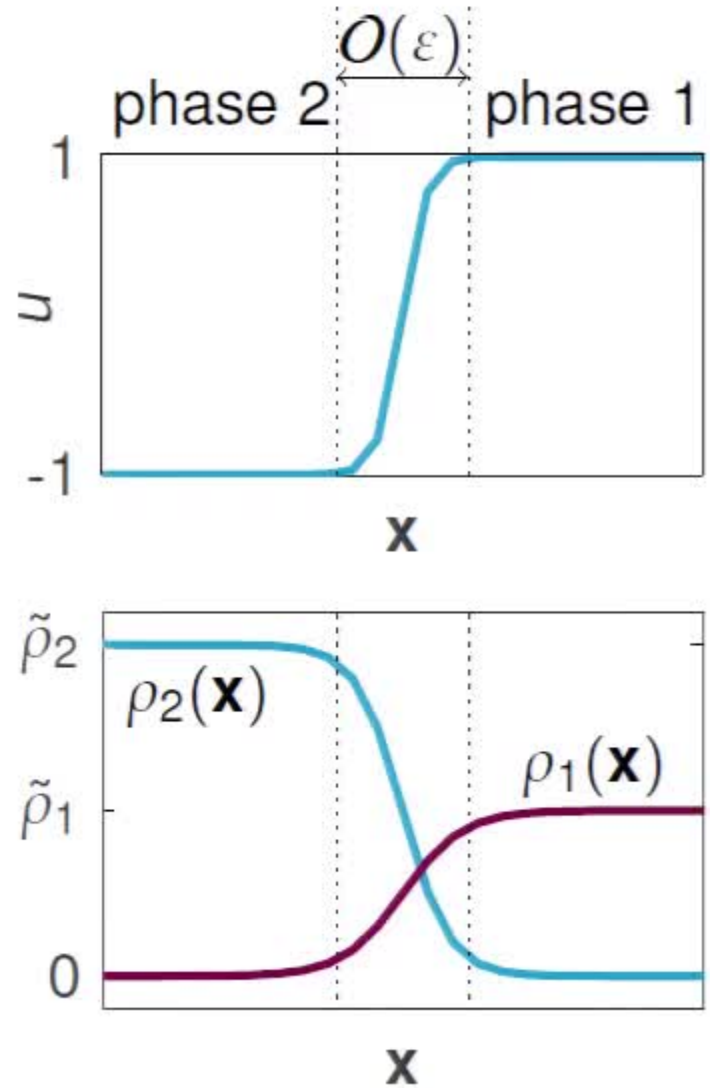
- rising bubble / falling droplet
- mixing of fluids in a driven cavity
- spinodal decomposition under shear
- Rayleigh–Taylor instability

Cahn–Hilliard Model

- continuous order-parameter u indicating the two phases

$$u(\mathbf{x}) = \frac{\rho_1(\mathbf{x})}{\tilde{\rho}_1} - \frac{\rho_2(\mathbf{x})}{\tilde{\rho}_2}$$

$$\in \begin{cases} \{-1\} & \text{if } \mathbf{x} \text{ in phase 2} \\ (-1,1) & \text{if } \mathbf{x} \text{ in interface} \\ \{1\} & \text{if } \mathbf{x} \text{ in phase 1} \end{cases}$$



- interface of small thickness $\mathcal{O}(\varepsilon)$
- mixing inside the interface

Diffuse Interface Approach

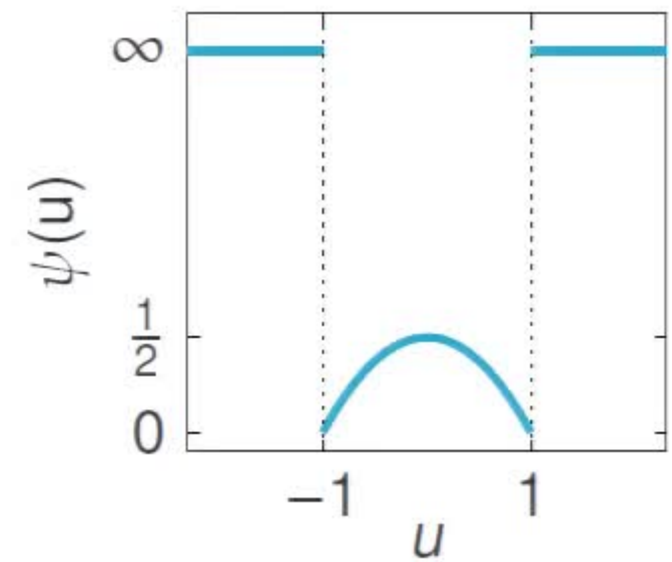
Energy Functional

- the evolution of u is driven by the minimization of

$$\mathcal{E}(u) = \int_\Omega \left[\frac{\sigma\varepsilon}{2} |\nabla u|^2 + \frac{\sigma}{\varepsilon}\psi(u) \right] \mathrm{d}\mathbf{x}$$

- double-obstacle potential

$$\psi(u) = \begin{cases} \frac{1}{2}(1-u^2) & \text{if } u \in [-1,1] \\ \infty & \text{else} \end{cases}$$



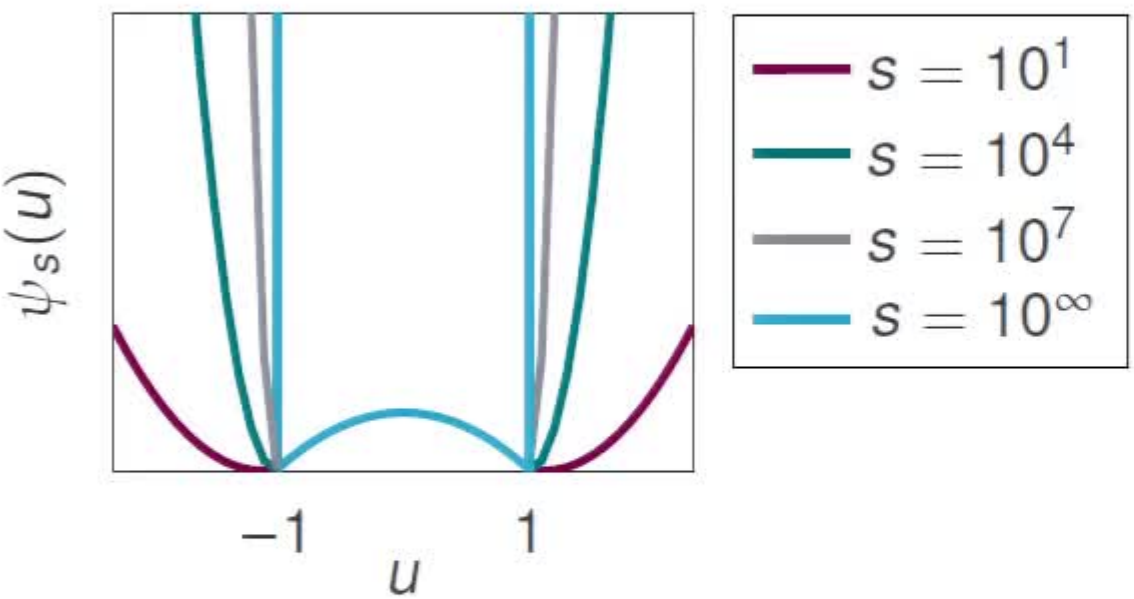
Regularized Potential

[Hintermüller/Hinze/Tber '11]

Relaxation by Moreau–Yosida regularization:

$$\lambda(u) = \max(0, u-1) + \min(0, u+1)$$

$$\psi_s(u) = \frac{1}{2}(1 - u^2 + s\lambda^2(u)) \qquad (s \to \infty)$$



Diffuse Interface Approach

Cahn–Hilliard Part

Convective Cahn–Hilliard equations

$$\begin{cases} \mathbf{v} \cdot \nabla u + \partial_t u &= \operatorname{div}(m \nabla w) \\ w &= -\sigma \varepsilon \Delta u + \sigma \varepsilon^{-1} \psi_s'(u) \end{cases}$$

- w chemical potential
- $m(u)$ mobility
- σ surface tension
- ε interfacial width
- $\mathbf{v}$ velocity

Boundary conditions

- $\nabla w \cdot \mathbf{n} = 0 \rightsquigarrow$ no diffusion through boundary
- $\nabla u \cdot \mathbf{n} = 0 \rightsquigarrow$ interface is orthogonal to the boundary

Navier–Stokes Part

Navier–Stokes equation + surface tension force

$$\begin{cases} \rho\partial_t \mathbf{v} + ((\rho\mathbf{v} + J)\cdot\nabla)\mathbf{v} - \operatorname{div}(2\eta D\mathbf{v}) + \nabla p = \rho\mathbf{g} + w\nabla u \\ \operatorname{div}\mathbf{v} = 0 \end{cases}$$

- $\rho(u)$ density
- $\eta(u)$ viscosity
- $\mathbf{g}$ gravitation
- $2D\mathbf{v} = \nabla\mathbf{v} + (\nabla\mathbf{v})^T$ strain tensor
- $J = -\frac{\tilde{\rho}_2 - \tilde{\rho}_1}{2} m(u)\nabla w$

Boundary conditions

- $\mathbf{v} = \mathbf{f}$ with $\mathbf{f}\cdot\mathbf{n} = 0$

Coupled System

[Abels/Garcke/Grün '12]

Cahn–Hilliard/Navier–Stokes system

$$
\begin{cases}
\rho\partial_t \mathbf{v} + ((\rho\mathbf{v} + J)\cdot\nabla)\mathbf{v} - \mathrm{div}(2\eta D\mathbf{v}) + \nabla p &= \rho\mathbf{g} + w\nabla u \\
\mathrm{div}\,\mathbf{v} &= 0 \\
\mathbf{v}\cdot\nabla u + \partial_t u &= \mathrm{div}(m\nabla w) \\
w &= -\sigma\varepsilon\Delta u + \sigma\varepsilon^{-1}\psi_s'(u)
\end{cases}
$$

- $w\nabla u$ capillary force
- $\mathbf{v}\cdot\nabla u$ convection term
- $J = -\frac{\tilde{\rho}_2-\tilde{\rho}_1}{2} m(u)\nabla w$ crucial for thermodynamical consistency

Discretization

[Garcke/Hinze/Kahle '15]

- thermodynamical consistent time discrete scheme
- adaptive spatial discretization
  $\rightsquigarrow$ thermodynamical consistency is conserved
- Taylor-Hood LBB-stable $P2 - P1$ finite elements for the velocity-pressure field
- $P1$ finite elements for the phase field and chemical potential

Fully Coupled CH/NS System

$$\mathcal{A}\mathbf{x} = \left(\begin{array}{ccc|cc} F_{11} & F_{12} & B_1^T & 0 & I_1 \\ F_{21} & F_{22} & B_2^T & 0 & I_2 \\ B_1 & B_2 & 0 & 0 & 0 \\ \hline T_1 & T_2 & 0 & C_{11} & C_{12} \\ 0 & 0 & 0 & C_{21} & C_{22} \end{array}\right) \begin{pmatrix} \delta v_1 \\ \delta v_2 \\ \delta p \\ \delta u \\ \delta w \end{pmatrix} = \begin{pmatrix} r_{v_1} \\ r_{v_2} \\ r_p \\ r_u \\ r_w \end{pmatrix}$$

- F discrete convection-diffusion operator
- B negative discrete divergence operator
- I interfacial force coupling
- T interfacial transport coupling
- C_{12} mobility dependent diffusion operator
- C_{21} diffusion operator + regularization

Optimal Preconditioning

Non-singular $(1,1)$ block (as in Navier–Stokes)

$$\mathcal{A} = \begin{pmatrix} F & B^T \\ B & 0 \end{pmatrix} \qquad \mathcal{P} = \begin{pmatrix} F & B^T \\ 0 & BF^{-1}B^T \end{pmatrix}$$

[MURPHY/GOLUB/WATHEN '00] showed exactly two eigenvalues ± 1.

Non-singular $(1,1)$ block

$$\mathcal{A} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \qquad \mathcal{P} = \begin{pmatrix} A & B \\ 0 & D - CA^{-1}B^T \end{pmatrix}$$

[IPSEN '01] showed exactly two eigenvalues ± 1.

Linear Systems and Preconditioning

Navier–Stokes Subproblem

$$\mathcal{A}_{NS} = \begin{pmatrix} F & B^T \\ B & 0 \end{pmatrix}$$

- F discrete convection-diffusion operator
- B negative discrete divergence operator

[Elman/Silvester/Wathen '05] showed

$$\mathcal{P}_{NS} = \begin{pmatrix} F & B^T \\ 0 & \hat{S}_{NS} \end{pmatrix} \qquad \hat{S}_{NS} = A_p F_p^{-1} Q_p$$

as a good approximation to the Schur complement preconditioner.

- A_p pressure space Laplacian
- F_p pressure space convection-diffusion operator
- Q_p pressure space mass matrix

Cahn–Hilliard Subproblem

$$\mathcal{A}_{CH} = \begin{pmatrix} M & -\varepsilon K - sGMG + \frac{1}{\varepsilon}M \\ \tau K & M \end{pmatrix} = \begin{pmatrix} M & -L \\ \tau K & M \end{pmatrix}$$

- M mass matrix
- K stiffness matrix
- G diagonal penalization matrix
- τ time step

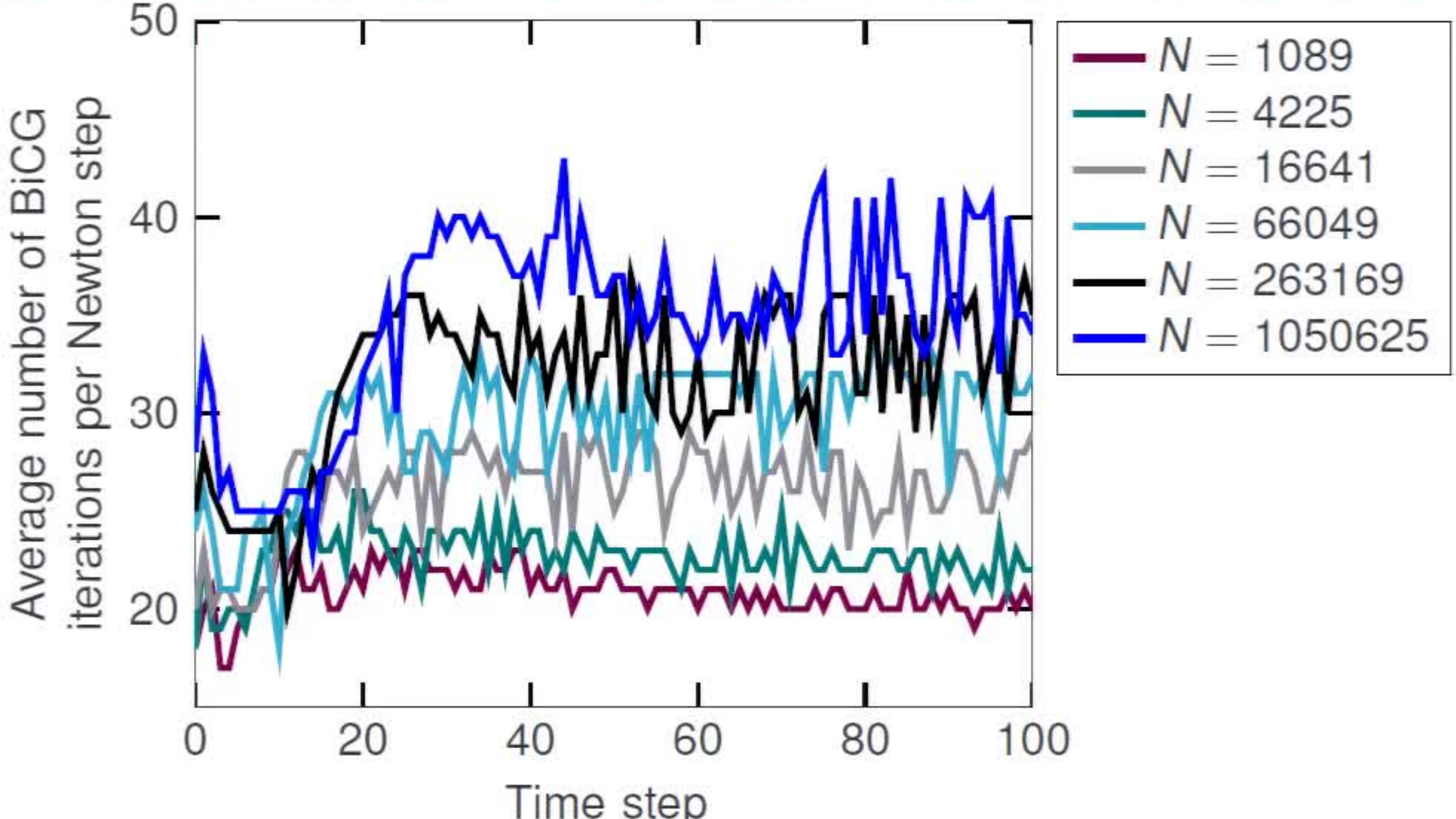
[Bosch/Stoll/Benner '14] showed

$$\mathcal{P}_{NS} = \begin{pmatrix} M & 0 \\ \tau K & -\hat{S}_{CH} \end{pmatrix} \qquad \hat{S}_{CH} = (M + \sqrt{\tau}K)M^{-1}(M + \sqrt{\tau}L)$$

as a good approximation to the Schur complement preconditioner.

Linear Systems and Preconditioning

BiCG Iteration Numbers for Different Uniform Meshes



CH/NS Preconditioner

$$\mathcal{A} = \left(\begin{array}{ccc|cc} F_{11} & F_{12} & B_1^T & 0 & I_1 \\ F_{21} & F_{22} & B_2^T & 0 & I_2 \\ B_1 & B_2 & 0 & 0 & 0 \\ \hline T_1 & T_2 & 0 & C_{11} & C_{12} \\ 0 & 0 & 0 & C_{21} & C_{22} \end{array}\right)$$

$$\mathcal{P} = \left(\begin{array}{ccc|cc} F_{11} & 0 & B_1^T & 0 & I_1 \\ 0 & F_{22} & B_2^T & 0 & I_2 \\ 0 & 0 & -\hat{S}_{NS} & 0 & 0 \\ \hline 0 & 0 & 0 & C_{21} & C_{22} \\ 0 & 0 & 0 & 0 & -\hat{S}_{CH} \end{array}\right)$$

CH/NS Preconditioner

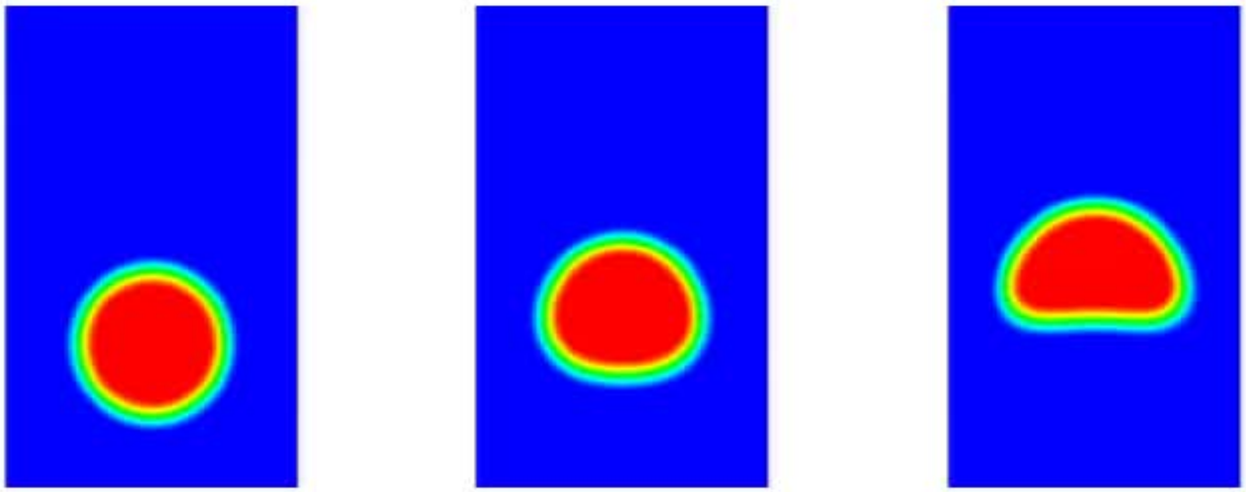
$$\mathcal{P} = \left(\begin{array}{ccc|cc} F_{11} & 0 & B_1^T & 0 & I_1 \\ 0 & F_{22} & B_2^T & 0 & I_2 \\ 0 & 0 & -\hat{S}_{NS} & 0 & 0 \\ \hline 0 & 0 & 0 & C_{21} & C_{22} \\ 0 & 0 & 0 & 0 & -\hat{S}_{CH} \end{array}\right)$$

$$S_{NS} = BF^{-1}B^T \qquad S_{CH} = C_{12} - C_{11}C_{21}^{-1}C_{22}$$

$$\hat{S}_{NS} = A_p F_p^{-1} Q_p \qquad \hat{S}_{CH} = S_A C_{21}^{-1} S_B = \left(\tau^{-1}C_{12} + C_{11}\right) C_{21}^{-1} \left(\tau C_{21} - C_{22}\right)$$

- F_{11}^{-1}, F_{22}^{-1} A_p^{-1} C_{21}^{-1}, S_A^{-1}, S_B^{-1} via AMG (library `HSL_MI20`)
- Q_p^{-1} via lumping

Rising Bubble



We fix:

$\tilde{\rho}_2 = 100$, $\tilde{\eta}_1 = 10$, $\tilde{\eta}_2 = 1$, $s = 10^6$, $\sigma = 15.6$

We vary:

h, $\tilde{\rho}_1 \rightsquigarrow \text{Re}$, ϵ, τ, m

Rising Bubble - Vary Mesh

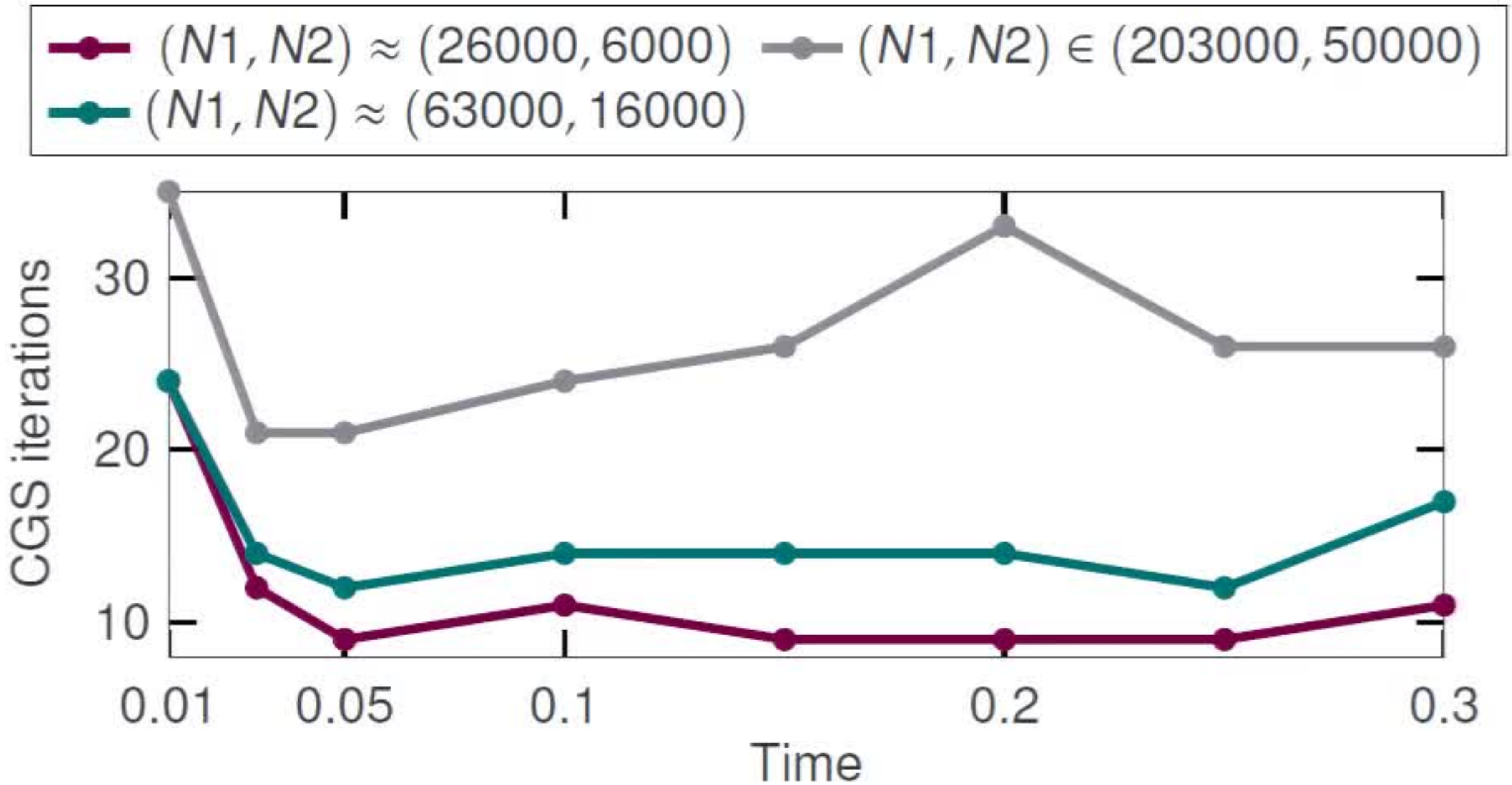
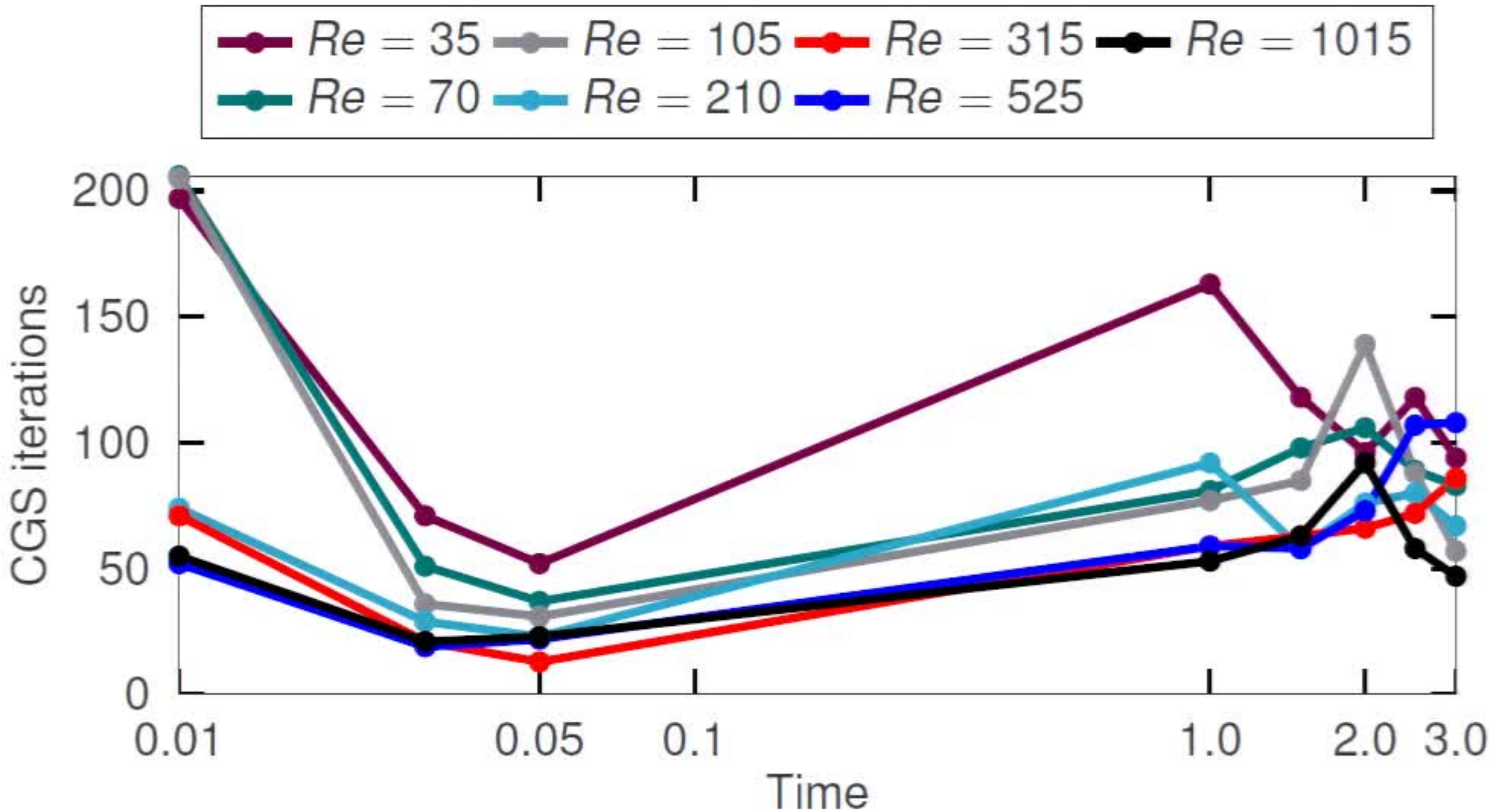


Figure : Vary the mesh, fix $\varepsilon = 0.04$, $\tau = 1.25 \cdot 10^{-4}$, $m = 4 \cdot 10^{-5}$, $\tilde{\rho}_1 = 1000$.

Numerical Results

Rising Bubble - Vary Density / Reynolds Number



Rising Bubble - Vary Mesh, Interface and Time Step Simultaneously