Preconditioning for Two-Phase Flows

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Jointly with Martin Stoll (moving to TU Chemnitz) and Christian Kahle (TU Munich).

[ABELS/GARCKE/GRÜN '12] proposed a diffuse interface model for incompressible two-phase flows with different densities.



[GARCKE/HINZE/KAHLE '16] developed a thermodynamically consistent discretization scheme for that model.

- Fully iterative solution of the large and sparse linear systems.
- Development of robust preconditioners.

two-phase flow



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- two-phase flow
- two immiscible, incompressible viscous fluids



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- different physical properties



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- different physical properties
 - densities $\tilde{\rho}_1$, $\tilde{\rho}_2$
 - viscosities $\tilde{\eta}_1$, $\tilde{\eta}_2$

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two-phase flow

- two immiscible, incompressible viscous fluids
- different physical properties
 - densities $\tilde{\rho}_1$, $\tilde{\rho}_2$
 - viscosities η
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 ₂
 - diffuse interface model

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two-phase flow

- two immiscible, incompressible viscous fluids
- different physical properties
 - densities $\tilde{\rho}_1$, $\tilde{\rho}_2$
 - viscosities η
 ₁, η
 ₂
- diffuse interface model
 - to cope with topological changes

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 continuous order-parameter u indicating the two phases



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



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$$\in \left\{ \begin{array}{ll} \{-1\} & \text{if } \textbf{x} \text{ in phase 2} \\ (-1,1) & \text{if } \textbf{x} \text{ in interface} \\ \{1\} & \text{if } \textbf{x} \text{ in phase 1} \end{array} \right.$$



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■ interface of small thickness $O(\varepsilon)$



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interface of small thickness O(ε)
 mixing inside the interface



Cahn–Hilliard Part

Cahn–Hilliard equations

$$\begin{aligned} \partial_t u &= \operatorname{div}(m\nabla w) \\ w &= -\sigma \varepsilon \Delta u + \sigma \varepsilon^{-1} \psi'_s(u) \end{aligned}$$

- w chemical potential
- \blacksquare *m*(*u*) mobility
- σ surface tension
- ε interfacial width
- $\psi_s(u) = \frac{1}{2}(1-u^2) + \frac{s}{2}(\max^2(0,u-1) + \min^2(0,u+1))$
- *s* regularization parameter

■ Boundary conditions
 ■ ∇w · n = 0
 ■ ∇u · n = 0

Convective Cahn–Hilliard equations

$$\mathbf{v} \cdot \nabla u + \partial_t u = \operatorname{div}(m \nabla w)$$
$$w = -\sigma \varepsilon \Delta u + \sigma \varepsilon^{-1} \psi'_{\mathsf{s}}(u)$$

- w chemical potential
- m(u) mobility
- σ surface tension
- ε interfacial width
- $\psi_s(u) = \frac{1}{2}(1-u^2) + \frac{s}{2}(\max^2(0,u-1) + \min^2(0,u+1))$
- *s* regularization parameter

v velocity

Boundary conditions
 ∇*w* · **n** = 0
 ∇*u* · **n** = 0

Navier–Stokes Part

Navier–Stokes equation

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

• $\rho(u)$ density

Boundary conditions
 v = f with f · n = 0

- $\eta(u)$ viscosity
- **g** gravitation
- **2**D**v** = ∇ **v** + $(\nabla$ **v** $)^T$ strain tensor

Navier–Stokes equation + surface tension force

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

$$\operatorname{div} \mathbf{v} = \mathbf{0}$$

• $\rho(u)$ density

Boundary conditions
 v = f with f · n = 0

- $\eta(u)$ viscosity
- **g** gravitation

■ 2D**v** =
$$\nabla$$
v + $(\nabla$ **v** $)^T$ strain tensor
■ J = $-\frac{\tilde{\rho}_2 - \tilde{\rho}_1}{2}m(u)\nabla w$

Cahn-Hilliard Navier-Stokes system by [ABELS/GARCKE/GRÜN '12]:

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

div $\mathbf{v} = 0$
 $\mathbf{v} \cdot \nabla u + \partial_t u = \operatorname{div}(m \nabla w)$
 $w = -\sigma \varepsilon \Delta u + \sigma \varepsilon^{-1} \psi'_s(u)$

- $w\nabla u$ capillary force
- **v** $\cdot \nabla u$ convection term

■ $J = -\frac{\tilde{\rho}_2 - \tilde{\rho}_1}{2} m(u) \nabla w$ crucial for thermodynamical consistency

thermodynamical consistent

- thermodynamical consistent
- adaptive spatial discretization

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- Taylor-Hood LBB-stable P2 P1 finite elements for the velocity-pressure field

- thermodynamical consistent
- adaptive spatial discretization
- 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 linear system

$$\mathcal{A}\mathbf{Z} = \begin{pmatrix} F_{11} & F_{12} & B_1^T & I_1 & 0\\ F_{21} & F_{22} & B_2^T & I_2 & 0\\ B_1 & B_2 & 0 & 0 & 0\\ \hline 0 & 0 & 0 & C_{11} & C_{12}\\ T_1 & T_2 & 0 & C_{21} & C_{22} \end{pmatrix} \begin{pmatrix} \delta v_1 \\ \delta v_2 \\ \delta p \\ \delta w \\ \delta u \end{pmatrix} = \begin{pmatrix} r_{v_1} \\ r_{v_2} \\ r_p \\ r_w \\ r_u \end{pmatrix}$$

- F discrete convection-diffusion operator
- B negative discrete divergence operator
- I interfacial force coupling
- T interfacial transport coupling
- C₁₁, C₂₂ mass matrices
- **\Box** C₁₂ diffusion operator + regularization
- C₂₁ mobility dependent diffusion operator

Outer Preconditioner

For our original problem with

$$\mathcal{A} = \begin{pmatrix} F_{11} & F_{12} & B_1^T & I_1 & 0 \\ F_{21} & F_{22} & B_2^T & I_2 & 0 \\ B_1 & B_2 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & C_{11} & C_{12} \\ T_1 & T_2 & 0 & C_{21} & C_{22} \end{pmatrix} = \left(\begin{array}{c|c} \mathcal{A}_{NS} & C_I \\ \hline C_T & \mathcal{A}_{CH} \end{array} \right),$$

we consider the right preconditioned matrix \mathcal{RP}_{out}^{-1} with

$$\mathcal{P}_{out} = \left(\begin{array}{c|c} \hat{\mathcal{A}}_{NS} & C_{I} \\ \hline 0 & \hat{S} \end{array}\right)$$

where $\hat{\mathcal{A}}_{NS} \approx \mathcal{A}_{NS}$ and $\hat{\mathcal{S}} \approx \mathcal{S} = \mathcal{A}_{CH} - C_T \mathcal{A}_{NS}^{-1} C_I$.

For any nonsingular matrix of the form

$$\mathcal{K} = \left(egin{array}{cc} \mathsf{A} & \mathsf{B} \\ \mathsf{C} & \mathsf{D} \end{array}
ight)$$
 ,

as our coupled problem, [Murphy/Golub/Wathen '00], [IPSEN '01] showed exactly one eigenvalue at 1 for the preconditioned system $\mathcal{KP}_{\mathcal{K}}^{-1}$ with

$$\mathcal{P}_{\mathcal{K}} = \left(\begin{array}{cc} A & B \\ 0 & D - CA^{-1}B^{T} \end{array}\right) = \left(\begin{array}{cc} A & B \\ 0 & S \end{array}\right).$$

For our original problem with

$$\mathcal{A} = \begin{pmatrix} F_{11} & F_{12} & B_1^T & I_1 & 0 \\ F_{21} & F_{22} & B_2^T & I_2 & 0 \\ B_1 & B_2 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & C_{11} & C_{12} \\ T_1 & T_2 & 0 & C_{21} & C_{22} \end{pmatrix} = \left(\begin{array}{c|c} \mathcal{A}_{NS} & C_I \\ \hline C_T & \mathcal{A}_{CH} \end{array} \right),$$

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where $\hat{\mathcal{A}}_{NS} \approx \mathcal{A}_{NS}$ and $\hat{\mathcal{S}} \approx \mathcal{S} = \mathcal{A}_{CH} - C_T \mathcal{A}_{NS}^{-1} C_I$.

Practical Preconditioner for \mathcal{R}_{NS}

For the Navier–Stokes problem

$$\mathcal{A}_{NS} = \left(egin{array}{cc} \mathbf{F} & \mathbf{B}^T \ \mathbf{B} & \mathbf{0} \end{array}
ight),$$

[Elman/Silvester/Wathen '05] showed

$$\hat{\mathcal{A}}_{NS} = \begin{pmatrix} \hat{\mathbf{F}} & \mathbf{B}^{T} \\ \mathbf{0} & \hat{S}_{NS} \end{pmatrix} \qquad \hat{S}_{NS} = A_{p} F_{p}^{-1} Q_{p}$$

as a good practical approximation, where

- A_p pressure space Laplacian
- \blacksquare *F*_p pressure space convection-diffusion operator
- \blacksquare Q_p pressure space mass matrix

For our original problem with

$$\mathcal{A} = \begin{pmatrix} F_{11} & F_{12} & B_1^T & I_1 & 0 \\ F_{21} & F_{22} & B_2^T & I_2 & 0 \\ B_1 & B_2 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & C_{11} & C_{12} \\ T_1 & T_2 & 0 & C_{21} & C_{22} \end{pmatrix} = \left(\begin{array}{c|c} \mathcal{A}_{NS} & C_I \\ \hline C_T & \mathcal{A}_{CH} \end{array} \right),$$

we consider the right preconditioned matrix \mathcal{RP}_{out}^{-1} with

$$\mathcal{P}_{out} = \left(\begin{array}{c|c} \hat{\mathcal{A}}_{NS} & C_{I} \\ \hline 0 & \hat{S} \end{array}\right)$$

where $\hat{\mathcal{A}}_{NS} \approx \mathcal{A}_{NS}$ and $\hat{\mathcal{S}} \approx \mathcal{S} = \mathcal{A}_{CH} - C_T \mathcal{A}_{NS}^{-1} C_I$.

Preconditioner for the Schur complement S

For

$$\mathcal{A} = \left(\begin{array}{c|c} \mathcal{A}_{\text{NS}} & C_{1} \\ \hline \\ C_{\text{T}} & \mathcal{A}_{\text{CH}} \end{array} \right) \qquad \mathcal{P}_{\text{out}} = \left(\begin{array}{c|c} \hat{\mathcal{A}}_{\text{NS}} & C_{1} \\ \hline \\ 0 & \hat{\mathcal{S}} \end{array} \right)$$

Preconditioner for the Schur complement S

For

$$\mathcal{A} = \left(\begin{array}{c|c} \mathcal{A}_{NS} & C_{I} \\ \hline C_{T} & \mathcal{A}_{CH} \end{array} \right) \qquad \mathcal{P}_{out} = \left(\begin{array}{c|c} \hat{\mathcal{A}}_{NS} & C_{I} \\ \hline 0 & \hat{S} \end{array} \right)$$

we have that

$$S = \mathcal{A}_{CH} - C_T \mathcal{A}_{NS}^{-1} C_H$$
$$\approx \mathcal{A}_{CH} - C_T \hat{\mathcal{A}}_{NS}^{-1} C_H$$
$$= \mathcal{A}_{CH}$$
$$= \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}.$$

To solve with the Schur complement approximation

$$\mathcal{A}_{CH} = \left(egin{array}{cc} C_{11} & C_{12} \ C_{21} & C_{22} \end{array}
ight) pprox \mathcal{S} \, ,$$

we apply preconditioned GMRES as inner iteration, with the inner preconditioner

$$\mathcal{P}_{in} = \left(egin{array}{cc} C_{11} & C_{12} \ 0 & -\hat{S}_{CH} \end{array}
ight).$$

In order to approximate the Schur complement

$$S_{CH} = C_{22} - C_{21}C_{11}^{-1}C_{12}$$
,

we follow the matching strategy, proposed by [PEARSON/WATHEN '12]. We construct an approximation

$$\hat{S}_{CH} = (C_{11} + \alpha C_{21})C_{11}^{-1}(C_{11} - \beta C_{12})$$

= $C_{22} - \alpha\beta C_{21}C_{11}^{-1}C_{12} + \alpha C_{21} - \beta C_{12}$

with $\alpha, \beta > 0$ being chosen such that the exact Schur complement is captured as close as possible; see [B./KAHLE/STOLL '17].

Iteration Numbers



- Preconditioning is essential.
- Many well-studied ingredients can be used.
- Numerically robustness w.r.t. the mesh size and Reynolds number (here). In our paper also w.r.t. other parameters.

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THANK YOU!