Sparse Days June 5–6, 2014 CERFACS, Toulouse

## Preconditioning for various Cahn–Hilliard systems

#### Jessica Bosch Martin Stoll

Max Planck Institute for Dynamics of Complex Technical Systems Numerical Linear Algebra for Dynamical Systems Magdeburg, Germany



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Multi Phases

Linear Systems and Preconditioning

Numerical Results







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### Two Phases Two-Phase Structure





•  $\Omega \subset \mathbb{R}^d, d \in \{1, 2, 3\}$ 



- $u: \Omega \times (0, T) \rightarrow \mathbb{R}$  concentration
- $u \in [-1, 1]$

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### Two Phases Energy Functional

$$\mathcal{E}(u) = \int_{\Omega} \frac{\varepsilon}{2} |\nabla u|^2 + \frac{1}{\varepsilon} \psi(u) \,\mathrm{d}\mathbf{x}$$

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### Two Phases Energy Functional

$$\mathcal{E}(u) = \int_{\Omega} \frac{\varepsilon}{2} |\nabla u|^2 + \frac{1}{\varepsilon} \psi(u) \, \mathrm{d} \mathbf{x}$$



$$\psi(u) = \frac{1}{4}(u^2 - 1)^2$$

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## Two Phases



$$\mathcal{E}(u) = \int_{\Omega} \frac{\varepsilon}{2} |\nabla u|^2 + \frac{1}{\varepsilon} \psi(u) \,\mathrm{d}\mathbf{x}$$



Smooth potential

$$\psi(u) = \frac{1}{4}(u^2 - 1)^2$$



### Nonsmooth potential

$$\psi(u) = \begin{cases} \frac{1}{2}(1-u^2) & \text{if } |u| \le 1, \\ \infty & \text{otherwise} \end{cases}$$
$$= \psi_0(u) + I_{[-1,1]}(u)$$

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### Two Phases Moreau–Yosida Regularization

$$\mathcal{E}(u) = \int_{\Omega} \frac{\varepsilon}{2} |\nabla u|^2 + \frac{1}{\varepsilon} \left( \psi_0(u) + I_{[-1,1]}(u) \right) \, \mathrm{d}\mathbf{x}$$

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### Two Phases Moreau–Yosida Regularization

$$\mathcal{E}(u) = \int_{\Omega} \frac{\varepsilon}{2} |\nabla u|^2 + \frac{1}{\varepsilon} \left( \psi_0(u) + I_{[-1,1]}(u) \right) d\mathbf{x}$$

$$\downarrow$$

$$\vartheta_{\nu}(u_{\nu}) \coloneqq \frac{1}{2\nu} \left( |\max(0, u_{\nu} - 1)|^2 + |\min(0, u_{\nu} + 1)|^2 \right)$$

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### Two Phases Moreau–Yosida Regularization

 $\mathcal{E}(u) = \int_{\Omega} \frac{\varepsilon}{2} |\nabla u|^2 + \frac{1}{\varepsilon} \left( \psi_0(u) + I_{[-1,1]}(u) \right) \, \mathrm{d}\mathbf{x}$  $\vartheta_{\nu}(u_{\nu}) \coloneqq \frac{1}{2\nu} \left( |\max(0, u_{\nu} - 1)|^2 + |\min(0, u_{\nu} + 1)|^2 \right)$  $\mathcal{E}_{\nu}(u_{\nu}) = \int_{\Omega} \frac{\varepsilon}{2} |\nabla u_{\nu}|^2 + \frac{1}{\varepsilon} \psi_0(u_{\nu}) + \vartheta_{\nu}(u_{\nu}) \,\mathrm{d}\mathbf{x}$ 



 $\partial_t u(t) = -\operatorname{grad}_{H^{-1}} \mathcal{E}(u(t))$ 

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### Two Phases Regularized Subproblem

$$\partial_t u(t) = -\operatorname{grad}_{H^{-1}} \mathcal{E}(u(t))$$

### System of two coupled PDEs

$$\partial_t u_{\nu} = \Delta w_{\nu}$$
$$w_{\nu} = -\varepsilon \Delta u_{\nu} + \frac{1}{\varepsilon} \psi'_0(u_{\nu}) + \theta_{\nu}(u_{\nu})$$
$$\nabla u_{\nu} \cdot \mathbf{n} = \nabla w_{\nu} \cdot \mathbf{n} = 0 \quad \text{on } \partial \Omega$$

Numerical Results



### Two Phases Regularized Subproblem



### System of two coupled PDEs

$$\partial_t u_{\nu} = \Delta w_{\nu}$$
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$$\nabla u_{\nu} \cdot \mathbf{n} = \nabla w_{\nu} \cdot \mathbf{n} = 0 \quad \text{on } \partial \Omega$$

$$\theta_{\nu}(u_{\nu}) \coloneqq \frac{1}{\nu} \left( \max\left(0, u_{\nu} - 1\right) + \min\left(0, u_{\nu} + 1\right) \right)$$

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### **Black-White Inpainting**

Idea



Original Cahn-Hilliard.

Inpainting version.

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J. Bosch, Preconditioning for various Cahn–Hilliard systems 8/27

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## **Black-White Inpainting**

Idea





Original image *f* with inpainting domain D.

Inpainted image.

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## **Black-White Inpainting**

Idea





Original image *f* with inpainting domain D.

Inpainted image.

$$\omega(x) = \begin{cases} 0 & \text{if } x \in D, \\ \omega_0 & \text{if } x \in \Omega \setminus D \end{cases}$$

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### **Black-White Inpainting**

#### Damaged Zebra Image



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### Multi Phases Multi-Phase Structure



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## Multi Phases

Modeling of Multi-Phase Systems

number of phases N

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## Multi Phases

Modeling of Multi-Phase Systems

- number of phases N
- vector-valued order parameter

$$\mathbf{u} = (u_1, \ldots, u_N)^T \colon \Omega \times (0, T) \to \mathbb{R}^N$$

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## Multi Phases

Modeling of Multi-Phase Systems

- number of phases N
- vector-valued order parameter

$$\mathbf{u} = (u_1, \ldots, u_N)^T \colon \Omega \times (0, T) \to \mathbb{R}^N$$

• 
$$u_i \in \begin{cases} \{0\} & \text{if phase } i \text{ is absent,} \\ (0, 1) & \text{if phase } i \text{ is present,} \\ \{1\} & \text{if only phase } i \text{ is present} \end{cases}$$

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### Multi Phases Modeling of Multi-Phase Systems

- number of phases N
- vector-valued order parameter

$$\mathbf{u} = (u_1, \ldots, u_N)^T \colon \Omega \times (0, T) \to \mathbb{R}^N$$

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admissible states belong to

$$\mathcal{G}^N \coloneqq \left\{ \mathbf{v} \in \mathbb{R}^N \left| \sum_{i=1}^N v_i = 1, v_i \ge 0 \ i = 1, \dots, N \right\} \right\}$$

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## Multi Phases

**Regularized Subproblems** 

### Systems of two coupled PDEs

$$\partial_t u_{\nu,i} = (L\Delta \mathbf{w}_{\nu})_i$$
$$w_{\nu,i} = -\varepsilon^2 \Delta u_{\nu,i} + \frac{\partial \psi_0(\mathbf{u}_{\nu})}{\partial u_{\nu,i}} + \theta_\nu(u_{\nu,i}) - \frac{1}{N} \sum_{j=1}^N \left( \theta_\nu(u_{\nu,j}) + \frac{\partial \psi_0(\mathbf{u}_{\nu})}{\partial u_{\nu,j}} \right)$$
$$V u_{\nu,i} \cdot \mathbf{n} = (L\nabla \mathbf{w}_{\nu})_i \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega$$

 $i = 1, \ldots, N$ 

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## Multi Phases

**Regularized Subproblems** 

### Systems of two coupled PDEs

$$\partial_t u_{\nu,i} = (L\Delta \mathbf{w}_{\nu})_i$$
$$w_{\nu,i} = -\varepsilon^2 \Delta u_{\nu,i} + \frac{\partial \psi_0(\mathbf{u}_{\nu})}{\partial u_{\nu,i}} + \theta_\nu(u_{\nu,i}) - \frac{1}{N} \sum_{j=1}^N \left( \theta_\nu(u_{\nu,j}) + \frac{\partial \psi_0(\mathbf{u}_{\nu})}{\partial u_{\nu,j}} \right)$$
$$7 u_{\nu,i} \cdot \mathbf{n} = (L\nabla \mathbf{w}_{\nu})_i \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega$$

*i* = 1, . . . , *N* 

Mobility: 
$$L = I - \frac{1}{N} \mathbf{1} \mathbf{1}^T$$
  $(L = I)$ 

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## Linear Systems and Preconditioning

**Final Steps to the Linear Systems** 

Time discretization:



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## Linear Systems and Preconditioning

- Time discretization:
  - Implicit Euler scheme → accurate



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## Linear Systems and Preconditioning

- Time discretization:
  - Implicit Euler scheme → accurate
  - Convexity splitting (semi-implicit) for inpainting  $\rightsquigarrow \tau > 0$



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## Linear Systems and Preconditioning

- Time discretization:
  - Implicit Euler scheme → accurate
  - Convexity splitting (semi-implicit) for inpainting  $\rightsquigarrow \tau > 0$
- Nonlinear systems: (Semismooth) Newton method



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## Linear Systems and Preconditioning

- Time discretization:
  - Implicit Euler scheme → accurate
  - Convexity splitting (semi-implicit) for inpainting  $\rightsquigarrow \tau > 0$
- Nonlinear systems: (Semismooth) Newton method
- Space discretization: Finite element method



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## Linear Systems and Preconditioning

**Optimal Preconditioners** 

$$\mathcal{K} = \left(\begin{array}{cc} \mathsf{A} & -\mathsf{B} \\ \mathsf{C} & \mathsf{D} \end{array}\right)$$

- A nonsingular
- Schur complement  $S = D + CA^{-1}B$



Linear Systems and Preconditioning

**Optimal Preconditioners** 

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

• Schur complement  $S = D + CA^{-1}B$ 

$$\mathcal{P} = \left( \begin{array}{cc} \mathbf{A} & \mathbf{0} \\ \mathbf{C} & -\hat{\mathbf{S}} \end{array} \right)$$

$$\hat{S} = S$$
:  
 $\Lambda(\mathcal{P}^{-1}\mathcal{K}) = \{1, -1\}$ 

[MURPHY/GOLUB/WATHEN '00]





Linear Systems and Preconditioning

**Optimal Preconditioners** 

Schur complement 
$$S = D + CA$$

$$\mathcal{P} = \left( egin{array}{cc} A & 0 \\ C & -\hat{S} \end{array} 
ight)$$
 •  $\hat{S} = S$ :  
  $\wedge (\mathcal{P}^{-1}\mathcal{K}) = \{1, -1\}$ 

[MURPHY/GOLUB/WATHEN '00]

#### Goal

# Good and easy to compute approximation $\hat{S}$ of the Schur complement *S*.

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 $^{-1}B$ 

Multi Phases

Linear Systems and Preconditioning
Linear Cahn–Hilliard Systems

$$\mathcal{K} = \begin{pmatrix} I_N \otimes M & -\mathcal{B} \\ \alpha L_N \otimes K & I_N \otimes (\beta M + \gamma K) \end{pmatrix} \qquad \alpha, \beta > 0, \gamma \ge 0$$



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Linear Cahn–Hilliard Systems

$$\mathcal{K} = \begin{pmatrix} I_N \otimes M & -\mathcal{B} \\ \alpha L_N \otimes K & I_N \otimes (\beta M + \gamma K) \end{pmatrix} \qquad \alpha, \beta > 0, \gamma \ge 0$$

#### ${\mathcal B}$ contains the potential and penalty terms



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Linear Cahn-Hilliard Systems

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#### $\mathcal{B}$ contains the potential and penalty terms

- if bound constraint is violated, otherwise  $\begin{cases} \frac{1}{\nu} \\ 0 \end{cases}$



Linear Cahn-Hilliard Systems

$$\mathcal{K} = \begin{pmatrix} I_N \otimes M & -\mathcal{B} \\ \alpha L_N \otimes K & I_N \otimes (\beta M + \gamma K) \end{pmatrix} \qquad \alpha, \beta > 0, \gamma \ge 0$$

#### $\mathcal B$ contains the potential and penalty terms

if bound constraint is violated, otherwise  $\begin{cases} \frac{1}{\nu} \\ 0 \end{cases}$ 

#### **Two Phases**

- N = 1
- $\mathcal{B}$  indefinite
- $\gamma = 0$

#### Inpainting

● *N* = 1

•  $\mathcal{B}$  symmetric positive (semi-)definite



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#### Linear Systems and Preconditioning

Schur Complement Approximation – Scalar Problems

$$\mathcal{K} = \begin{pmatrix} M & -\mathcal{B} \\ \alpha K & \beta M + \gamma K \end{pmatrix}$$

$$\alpha,\beta>0,\gamma\geq 0$$

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#### Linear Systems and Preconditioning

Schur Complement Approximation – Scalar Problems

$$\mathcal{K} = \begin{pmatrix} M & -\mathcal{B} \\ \alpha K & \beta M + \gamma K \end{pmatrix}$$

$$\alpha, \beta > 0, \gamma \ge 0$$

The Schur complement

$$S = \beta M + \alpha K M^{-1} \mathcal{B} + \gamma K$$

is approximated by



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#### Linear Systems and Preconditioning

Schur Complement Approximation – Scalar Problems

$$\mathcal{K} = \begin{pmatrix} M & -\mathcal{B} \\ \alpha K & \beta M + \gamma K \end{pmatrix}$$

$$\alpha, \beta > 0, \gamma \ge 0$$

The Schur complement

$$\mathcal{S} = \beta \mathbf{M} + \alpha \mathbf{K} \mathbf{M}^{-1} \mathcal{B} + \gamma \mathbf{K}$$

is approximated by

$$\hat{\mathcal{S}} = \left(\sqrt{\beta}M + \sqrt{\alpha}K\right)M^{-1}\left(\sqrt{\beta}M + \sqrt{\alpha}\mathcal{B}\right)$$

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#### Linear Systems and Preconditioning

Schur Complement Approximation – Scalar Problems

$$\mathcal{K} = \begin{pmatrix} M & -\mathcal{B} \\ \alpha K & \beta M + \gamma K \end{pmatrix}$$

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is approximated by

$$\hat{S} = \left(\sqrt{\beta}M + \sqrt{\alpha}K\right)M^{-1}\left(\sqrt{\beta}M + \sqrt{\alpha}B\right)$$
$$= \beta M + \alpha K M^{-1}B + \sqrt{\alpha\beta}K + \sqrt{\alpha\beta}B.$$



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#### Linear Systems and Preconditioning

Schur Complement Approximation – Scalar Problems

$$\mathcal{K} = \begin{pmatrix} M & -\mathcal{B} \\ \alpha K & \beta M + \gamma K \end{pmatrix}$$

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#### Linear Systems and Preconditioning

Schur Complement Approximation – Scalar Problems

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#### Linear Systems and Preconditioning

Schur Complement Approximation – Scalar Problems

$$\mathcal{K} = \begin{pmatrix} M & -\mathcal{B} \\ \alpha K & \beta M + \gamma K \end{pmatrix}$$

$$\alpha, \beta > 0, \gamma \ge 0$$

The Schur complement

$$\mathcal{S} = \beta \mathbf{M} + \alpha \mathbf{K} \mathbf{M}^{-1} \mathcal{B} + \gamma \mathbf{K}$$

is approximated by



The shift  $\sqrt{\beta}M$  makes  $\left(\sqrt{\beta}M + \sqrt{\alpha}\mathcal{B}\right)$  positive definite.

Linear Multi-Phase Cahn–Hilliard Systems

For e.g. N = 3 phases,  $\mathcal{K}$  is given as

$$\mathcal{K} = \begin{pmatrix} M & 0 & 0 & -B_{11} & -B_2 & -B_3 \\ 0 & M & 0 & -B_1 & -B_{22} & -B_3 \\ 0 & 0 & M & -B_1 & -B_2 & -B_{33} \\ \hline \tau L_{1,1} K & \tau L_{1,2} K & \tau L_{1,3} K & M & 0 & 0 \\ \tau L_{1,2} K & \tau L_{2,2} K & \tau L_{2,3} K & 0 & M & 0 \\ \tau L_{1,3} K & \tau L_{2,3} K & \tau L_{3,3} K & 0 & 0 & M \end{pmatrix}.$$

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We need a Schur complement approximation of

 $S = I \otimes M + \tau (L \otimes K) (I \otimes M)^{-1} \mathcal{B}.$ 



Multi Phases

Linear Systems and Preconditionin

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Linear Multi-Phase Cahn–Hilliard Systems

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We need a Schur complement approximation of

 $\mathcal{S} = I \otimes M + \tau (L \otimes K) (I \otimes M)^{-1} \mathcal{B}.$ 

Smooth potential ~> 'simple'





Linear Multi-Phase Cahn–Hilliard Systems

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We need a Schur complement approximation of

 $\mathcal{S} = I \otimes M + \tau (L \otimes K) (I \otimes M)^{-1} \mathcal{B}.$ 

Smooth potential  $\rightarrow$  'simple'

Onstant Potential  $\rightsquigarrow$  penalty terms in every block of  $\mathcal{B}$ 



Multi Phase

Linear Systems and Precondition

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#### Linear Systems and Preconditioning

Smooth Potential – Approximation of the Block  ${\mathcal B}$ 

$$\mathcal{B} = \begin{pmatrix} B_{11} & B_2 & B_3 \\ B_1 & B_{22} & B_3 \\ B_1 & B_2 & B_{33} \end{pmatrix} \qquad (N = 3)$$



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#### Linear Systems and Preconditioning

Smooth Potential – Approximation of the Block  $\ensuremath{\mathcal{B}}$ 

$$\mathcal{B} = \begin{pmatrix} B_{11} & B_2 & B_3 \\ B_1 & B_{22} & B_3 \\ B_1 & B_2 & B_{33} \end{pmatrix} \qquad (N = 3)$$

The block  $\mathcal{B}$  is given for i = 1, ..., N as

$$F_i = \operatorname{diag}\left(3\left(u_i^{(k)}(\mathbf{x}_h)\right)^2 - 3u_i^{(k)}(\mathbf{x}_h) + \frac{1}{2}\right)$$



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#### Linear Systems and Preconditioning



Smooth Potential – Approximation of the Block  $\ensuremath{\mathcal{B}}$ 

$$\mathcal{B} = \begin{pmatrix} B_{11} & B_2 & B_3 \\ B_1 & B_{22} & B_3 \\ B_1 & B_2 & B_{33} \end{pmatrix} \qquad (N=3)$$

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$$B_{ii} = \varepsilon^2 K + \left(\frac{N-1}{N}\right) F_i M F_i$$

$$B_i = -\frac{1}{N}F_iMF_i$$

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#### Linear Systems and Preconditioning



Smooth Potential – Approximation of the Block  $\ensuremath{\mathcal{B}}$ 

$$\mathcal{B} = \begin{pmatrix} B_{11} & B_2 & B_3 \\ B_1 & B_{22} & B_3 \\ B_1 & B_2 & B_{33} \end{pmatrix} \qquad (N=3)$$

The block  $\mathcal{B}$  is given for i = 1, ..., N as

$$F_{i} = \text{diag}\left(3\left(u_{i}^{(k)}(\mathbf{x}_{h})\right)^{2} - 3u_{i}^{(k)}(\mathbf{x}_{h}) + \frac{1}{2}\right) \underset{\sim}{\overset{\leftarrow}{=}} (-2.5, 3.5)$$

$$B_{ii} = \varepsilon^2 K + \left(\frac{N-1}{N}\right) F_i M F_i$$

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#### Linear Systems and Preconditioning

Smooth Potential – Approximation of the Block  ${\mathcal B}$ 

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Smooth Potential – Approximation of the Block  ${\mathcal B}$ 

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#### Linear Systems and Preconditioning

Smooth Potential – Approximation of the Block  ${\mathcal B}$ 

$$\mathcal{B} = \begin{pmatrix} B_{11} & B_2 & B_3 \\ B_1 & B_{22} & B_3 \\ B_1 & B_2 & B_{33} \end{pmatrix} \qquad (N = 3) \qquad \hat{\mathcal{B}} = \begin{pmatrix} \hat{B} & 0 & 0 \\ 0 & \hat{B} & 0 \\ 0 & 0 & \hat{B} \end{pmatrix}$$

The block  $\mathcal{B}$  is given for i = 1, ..., N as

$$F_{i} = \text{diag}\left(3\left(u_{i}^{(k)}(\mathbf{x}_{h})\right)^{2} - 3u_{i}^{(k)}(\mathbf{x}_{h}) + \frac{1}{2}\right) \underset{\sim}{\overset{\leftarrow}{=}} (-2.5, 3.5)$$

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### Linear Systems and Preconditioning

Smooth Potential – Schur Complement Approximation

The Schur complement

$$S = I \otimes M + \tau (L \otimes K) (I \otimes M)^{-1} \mathcal{B}$$

is then approximated by



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### Linear Systems and Preconditioning

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The Schur complement

$$\mathcal{S} = I \otimes M + \tau (L \otimes K) (I \otimes M)^{-1} \mathcal{B}$$

is then approximated by

$$\hat{\mathcal{S}} = \left(\frac{N}{N-1}I \otimes M + \tau L \otimes K\right)(I \otimes M)^{-1}\left(\frac{N-1}{N}I \otimes M + \varepsilon^2 I \otimes K\right)$$

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$$= \left(\frac{N}{N-1}I \otimes M + \tau L \otimes K\right)(I \otimes M)^{-1}\hat{B}$$



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is then approximated by

$$\begin{split} \hat{\mathcal{S}} &= \Big(\frac{N}{N-1}I \otimes M + \tau L \otimes K\Big)(I \otimes M)^{-1}\Big(\frac{N-1}{N}I \otimes M + \varepsilon^2 I \otimes K\Big) \\ &= \Big(\frac{N}{N-1}I \otimes M + \tau L \otimes K\Big)(I \otimes M)^{-1}\hat{\mathcal{B}} \\ &= I \otimes M + \tau (L \otimes K)(I \otimes M)^{-1}\hat{\mathcal{B}} + \frac{\varepsilon^2 N}{N-1}I \otimes K. \end{split}$$



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### Linear Systems and Preconditioning

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is then approximated by

4

$$\hat{S} = \left(\frac{N}{N-1}I \otimes M + \tau L \otimes K\right)(I \otimes M)^{-1}\left(\frac{N-1}{N}I \otimes M + \varepsilon^2 I \otimes K\right)$$
$$= \left(\frac{N}{N-1}I \otimes M + \tau L \otimes K\right)(I \otimes M)^{-1}\hat{\mathcal{B}}$$
$$= I \otimes M + \tau (L \otimes K)(I \otimes M)^{-1}\hat{\mathcal{B}} + \frac{\varepsilon^2 N}{N-1}I \otimes K.$$

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### Linear Systems and Preconditioning

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$$\hat{S} = \overbrace{\left(\frac{N}{N-1}I \otimes M + \tau L \otimes K\right)}^{\mathsf{FFT} + \mathsf{AMG}} \underbrace{\left(L = I - \frac{1}{N}\mathbf{1}\mathbf{1}^{\mathsf{T}}\right)}_{\mathsf{AMG}} \underbrace{\mathsf{AMG}}_{\mathsf{AMG}}$$

$$= \underbrace{\left(\frac{N}{N-1}I \otimes M + \tau L \otimes K\right)}_{\mathsf{AMG}} (I \otimes M)^{-1} \widehat{\mathcal{B}}$$

$$= I \otimes M + \tau (L \otimes K)(I \otimes M)^{-1} \widehat{\mathcal{B}} + \frac{\varepsilon^2 N}{N-1}I \otimes K.$$

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## Linear Systems and Preconditioning

FFT based Preconditioner [STOLL '13]

$$\frac{N}{N-1}I \otimes M + \tau L \otimes K \Big) \mathbf{y} = \mathbf{g}$$
(1)



FFT based Preconditioner [STOLL '13]

$$\left(\frac{N}{N-1}I\otimes M+\tau L\otimes K\right)\mathbf{y}=\mathbf{g} \tag{1}$$

• 
$$L = F \operatorname{diag}(\lambda_1, \ldots, \lambda_N) F^H$$
 [Chen '87]





FFT based Preconditioner [STOLL '13]

$$\left(\frac{N}{N-1}I\otimes M+\tau L\otimes K\right)\mathbf{y}=\mathbf{g} \tag{1}$$

• 
$$L = F \operatorname{diag}(\lambda_1, \dots, \lambda_N) F^H$$
 [Chen '87]

apply FFT to (1)



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$$(F^{H} \otimes I) \left( \frac{N}{N-1} I \otimes M + \tau L \otimes K \right) (F \otimes I) (F^{H} \otimes I) \mathbf{y} = (F^{H} \otimes I) \mathbf{g}$$
(1)

- $L = F \operatorname{diag}(\lambda_1, \ldots, \lambda_N) F^H$  [Chen '87]
- apply FFT to (1)



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$$(F^{H} \otimes I) \left( \frac{N}{N-1} I \otimes M + \tau L \otimes K \right) (F \otimes I) (F^{H} \otimes I) \mathbf{y} = (F^{H} \otimes I) \mathbf{g}$$
(1)

• 
$$L = F \operatorname{diag}(\lambda_1, \ldots, \lambda_N) F^H$$
 [Chen '87]

equivalent block-diagonal system

$$\left(\frac{N}{N-1}I\otimes M+\tau \operatorname{diag}(\lambda_1,\ldots,\lambda_N)\otimes K\right)\tilde{\mathbf{y}}=\tilde{\mathbf{g}}.$$





Nonsmooth Potential – The Block  ${\mathcal B}$ 

$$\mathcal{B} = \begin{pmatrix} B_{11} & B_2 & B_3 \\ B_1 & B_{22} & B_3 \\ B_1 & B_2 & B_{33} \end{pmatrix} \qquad (N=3)$$



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Nonsmooth Potential – The Block  ${\mathcal B}$ 

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The block  $\mathcal{B}$  is given for i = 1, ..., N as

$$G_i = \operatorname{diag} \left( \begin{array}{cc} 1 & \operatorname{if} u_i^{(k)}(\mathbf{x}_h) < 0, \\ 0 & \operatorname{otherwise} \end{array} \right)$$



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Nonsmooth Potential – The Block  ${\mathcal B}$ 

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$$G_{i} = \operatorname{diag} \begin{pmatrix} 1 & \text{if } u_{i}^{(K)}(\mathbf{x}_{h}) < 0, \\ 0 & \text{otherwise} \end{pmatrix}$$
$$B_{ii} = \varepsilon^{2} K + \left(\frac{N-1}{N}\right) \left(\frac{1}{\nu} G_{i} M G_{i} - M\right)$$
$$B_{i} = -\frac{1}{N} \left(\frac{1}{\nu} G_{i} M G_{i} - M\right)$$



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## Linear Systems and Preconditioning

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$$B_{i} = -\frac{1}{N} \left(\frac{1}{\nu} G_{i} M G_{i} - M\right)$$

 $\nu \ll 1 \Rightarrow$  Cannot neglect this term!

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Nonsmooth Potential – Schur Complement Approximation

The Schur complement

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$$= I \otimes M + \tau(L \otimes K)(I \otimes M)^{-1}B + \frac{\sqrt{\tau}N}{N-1}B + \frac{\sqrt{\tau}(N-1)}{N}L \otimes K.$$



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is then approximated by

$$\hat{S} = \overbrace{\left(\frac{N}{N-1}I \otimes M + \sqrt{\tau}L \otimes K\right)}^{\text{FFT} + \text{AMG}} (I \otimes M)^{-1} \overbrace{\left(\frac{N-1}{N}I \otimes M + \sqrt{\tau}B\right)}^{\text{Jacobi + AMG}}$$
$$= I \otimes M + \tau (L \otimes K) (I \otimes M)^{-1} \mathcal{B} + \frac{\sqrt{\tau}N}{N-1} \mathcal{B} + \frac{\sqrt{\tau}(N-1)}{N} L \otimes K.$$

The shift with *M* makes the diagonal blocks of  $\left(\frac{N-1}{N}I \otimes M + \sqrt{\tau}\mathcal{B}\right)$  positive definite.

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## **Numerical Results**

**Two Phases – BiCG Iteration Numbers** 



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## **Numerical Results**



#### Smooth Multi-Phase Model – BiCG Iteration Numbers



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## **Numerical Results**

Nonsmooth Multi-Phase Model – BiCG Iteration Numbers



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## **Numerical Results**

**Results and Outlook** 

#### Results

• Smooth: Numerically mesh and phase independent preconditioners.

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## **Numerical Results**

**Results and Outlook** 

#### Results

- Smooth: Numerically mesh and phase independent preconditioners.
- Moreau–Yosida based solver for the handling of the nonsmoothness.

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## **Numerical Results**

**Results and Outlook** 

### Results

- Smooth: Numerically mesh and phase independent preconditioners.
- Moreau–Yosida based solver for the handling of the nonsmoothness.
- Nonsmooth: Outperforming preconditioned version compared to the unpreconditioned one.

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# **Numerical Results**

**Results and Outlook** 

#### Results

- Smooth: Numerically mesh and phase independent preconditioners.
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- More accurate results with the nonsmooth model.

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# **Numerical Results**

**Results and Outlook** 

### Results

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#### Outlook

• Proofs for the preconditioner.

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# **Numerical Results**

**Results and Outlook** 

### Results

- Smooth: Numerically mesh and phase independent preconditioners.
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# **Numerical Results**

**Results and Outlook** 

## Results

- Smooth: Numerically mesh and phase independent preconditioners.
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#### Outlook

- Proofs for the preconditioner.
- Nonsmooth: Enhanced Schur complement approximation?
- Grey/color inpainting.

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Multi Phases

#### Two Phases Different Potentials





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## Two Phases







#### Two Phases **Dumbbell in 3D**



- $\Omega = (-1, 1)^3$
- $\varepsilon = 0.03$
- $\tau = 5 \cdot 10^{-5}$
- $c_{max} = 10^{-5}$
- $h_0 = 2^{-5}$ •  $h_{\min} = \frac{\varepsilon \pi}{9}$ 
  - $h_{\rm max} = 10 \cdot h_{\rm min}$

(a) n = 0









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#### Moreau-Yosida Semismooth Newton (SSN) Solver in 1D

<b>C</b> max	$\ u_{c_{\max},h}-u_{\mathrm{ex},h}\ _2$	max. SSN\BiCG iterations	CPU time (s)
10 <sup>-3</sup>	2.46337 · 10 <sup>-2</sup>	2\14	0.34
10 <sup>-6</sup>	3.05118 · 10 <sup>−3</sup>	2\14	0.41
10 <sup>-9</sup>	3.06076 · 10 <sup>-3</sup>	2\14	0.50
10 <sup>-3</sup>	3.58987 · 10 <sup>-2</sup>	3\15	0.61
10 <sup>-6</sup>	9.32589 · 10 <sup>-4</sup>	3\16	0.87
10 <sup>-9</sup>	$9.31919 \cdot 10^{-4}$	3\16	1.00
10 <sup>-3</sup>	5.04977 · 10 <sup>-2</sup>	3\15	1.17
10 <sup>-6</sup>	6.92492 · 10 <sup>-4</sup>	3\16	1.80
10 <sup>-9</sup>	6.71485 · 10 <sup>-4</sup>	3\17	2.12
10 <sup>-3</sup>	7.10723 · 10 <sup>-2</sup>	3\15	2.17
10 <sup>-6</sup>	2.63167 · 10 <sup>-4</sup>	3\16	3.55
10 <sup>-9</sup>	$1.99167 \cdot 10^{-4}$	3\17	4.07
	$\begin{array}{c} C_{max} \\ 10^{-3} \\ 10^{-6} \\ 10^{-9} \\ 10^{-3} \\ 10^{-6} \\ 10^{-9} \\ 10^{-3} \\ 10^{-6} \\ 10^{-9} \\ 10^{-3} \\ 10^{-6} \\ 10^{-9} \end{array}$	$\begin{array}{c c} c_{max} &   u_{c_{max},h} - u_{ex,h}  _2 \\ \hline 10^{-3} & 2.46337 \cdot 10^{-2} \\ 10^{-6} & 3.05118 \cdot 10^{-3} \\ 10^{-9} & 3.06076 \cdot 10^{-3} \\ 10^{-3} & 3.58987 \cdot 10^{-2} \\ 10^{-6} & 9.32589 \cdot 10^{-4} \\ 10^{-9} & 9.31919 \cdot 10^{-4} \\ 10^{-3} & 5.04977 \cdot 10^{-2} \\ 10^{-6} & 6.92492 \cdot 10^{-4} \\ 10^{-9} & 6.71485 \cdot 10^{-4} \\ 10^{-3} & 7.10723 \cdot 10^{-2} \\ 10^{-6} & 2.63167 \cdot 10^{-4} \\ 10^{-9} & 1.99167 \cdot 10^{-4} \end{array}$	$\begin{array}{c c c c c c c c c c c c c c c c c c c $

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## **Two Phases**

Semi-Implicit Time Discretization and Large Time Steps



Figure: Initial state.

#### Exact solution

Small red circle vanishes at time  $t = 1.85 \cdot 10^{-3}$ .

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# Two Phases

Semi-Implicit Time Discretization and Large Time Steps



Figure: Semi-implicit Cahn–Hilliard evolution with different time steps  $\tau$ . The figure shows the solutions at time  $t = 3 \cdot 10^{-3}$ .

Remember: In the exact solution the small red circle vanishes at time  $t = 1.85 \cdot 10^{-3}$ .

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## **Black-White Inpainting**

Modified Cahn-Hilliard Model

$$\partial_t u(t) = -\operatorname{grad}_{H^{-1}} \mathcal{E}(u(t)) - \operatorname{grad}_{L^2} \mathcal{E}_2(u(t))$$

$$\mathcal{E}_2(u) = \int_{\Omega} \frac{\omega}{2} (f-u)^2 \,\mathrm{d}\mathbf{x}$$

#### Regularized modified Cahn-Hilliard subproblem

$$\partial_t u_{\nu} = \Delta \left( -\varepsilon \Delta u_{\nu} + \frac{1}{\varepsilon} \psi_0'(u_{\nu}) + \theta_{\nu}(u_{\nu}) \right) + \omega (f - u_{\nu})$$
$$\nabla u_{\nu} \cdot \mathbf{n} = \nabla (\Delta u_{\nu}) \cdot \mathbf{n} = 0 \quad \text{on } \partial \Omega$$

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## **Black-White Inpainting**



#### Three-Dimensional Space



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# **Black-White Inpainting**







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# **Black-White Inpainting**

Nonsmooth Potential – BiCG Iteration Numbers



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## **Black-White Inpainting**

**Comparison to Other Methods** 



#### Figure: Initial state.

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# **Black-White Inpainting**

**Comparison to Other Methods** 





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#### Black-White Inpainting FEM vs. FFT – Smooth Potential





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# **Black-White Inpainting**





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## **Black-White Inpainting**



#### FFT with Regularization





#### Multi Phases Final Steps to the Linear Systems

• Time discretization: Implicit Euler scheme

$$\tau < \frac{4\varepsilon^2}{\lambda_{\max}^2(A) \|L\|}$$
 (nonsmooth)  $\Rightarrow$  here:  $\tau < 4\varepsilon^2$ 

[BLOWEY/COPETTI/ELLIOTT '96]

Nonlinear systems: (Semismooth) Newton method

 $(\min(0, v))' \rightsquigarrow \chi_{\mathcal{A}(v)},$ 

where  $\mathcal{A}(v) \coloneqq \{ \mathbf{x} \in \Omega : v(\mathbf{x}) < 0 \}$ 

Space discretization: Finite element method



#### Multi Phases FFT based Preconditioner [STOLL '13]

We formulate each of the *N* complex valued systems to  $2 \times 2$  real valued block systems. As  $\lambda_1 = 0$  and  $\lambda_2 = \ldots = \lambda_N = 1$  we get two types

$$\begin{bmatrix} \frac{N}{N-1}M(+\tau K) & 0\\ 0 & \frac{N}{N-1}M(+\tau K) \end{bmatrix} \begin{bmatrix} \tilde{y}_r\\ \tilde{y}_c \end{bmatrix} = \begin{bmatrix} \tilde{g}_r\\ \tilde{g}_c \end{bmatrix}$$

which are solved with a fixed number of steps of

#### Inexact Uzawa method

$$\tilde{\mathbf{y}}^{(l+1)} = \tilde{\mathbf{y}}^{(l)} + \omega \mathcal{P}_1^{-1} \mathbf{r}^{(l)},$$

where  $\mathcal{P}_1$  is a block-diagonal AMG preconditioner.

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#### Multi Phases Evolution of Multi Phases



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Multi Phases



#### Multi Phases Smooth vs. Nonsmooth Evolution







n = 0

n = 20





*n* = 100
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## Multi Phases Smooth vs. Nonsmooth Evolution

			Time step	
		20	60	100
Min	Smooth	-0.02771	-0.02439	-0.02627
0	Nonsmooth	-1.186 · 10 <sup>-7</sup>	-1.172 · 10 <sup>-7</sup>	-1.178 · 10 <sup>-7</sup>
Max	Smooth	0.9764	1.001	0.9972
1	Nonsmooth	1	1	1

Table: Minimum and maximum values of the phase variable  $u_1$  in the smooth and nonsmooth model.

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## **Multi Phases**



## Nonsmooth Potential – BiCG Iteration Numbers



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## **Multi Phases**



