Robust BPX Solver for Cahn-Hilliard Equations

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1 Introduction

Since their introduction in the late 1950's, the Cahn-Hilliard equations have played an important role in understanding phase transition phenomena that is observed in materials. In particular, Cahn-Hilliard equations describe the process of phase separation in which a mixture of two materials separate or fuse to form pure material domains. The main purpose of these proceedings is to develop robust solvers for a well-known unconditionally stable time-stepping discretization.

Let $\Omega \subset \mathbb{R}^d$, $d \leq 3$, be a polygonal or polyhedral with boundary denoted by $\partial\Omega$. We focus on Cahn-Hilliard equations [5] with initial and boundary conditions defined as

$$u_t = \Delta w, \qquad x \in \Omega,\ t > 0, \tag{1a}$$

$$w = \Psi'(u) - \gamma \Delta u, \qquad x \in \Omega,\ t > 0, \tag{1b}$$

$$u(x,0) = u_0(x), \qquad x \in \Omega, \tag{1c}$$

$$\nabla u \cdot n = \nabla w \cdot n = 0, \qquad x \in \partial\Omega,\ t > 0, \tag{1d}$$

where u is the order parameter, such as concentration in a binary compound, with $u = \pm 1$ indicating pure states, $\Psi(u)$ is the potential function and $\gamma > 0$ is related to interfacial width between the two phases. n denotes the normal vector to $\partial\Omega$. In this article we consider the logarithmic nonlinear potential defined as

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$$\Psi(u) := \frac{\theta}{2}\big[(1+u)\ln(1+u) + (1-u)\ln(1-u)\big] + \frac{\theta_c}{2}(1-u^2), \quad 0 < \theta < \theta_c.$$

Following the splitting scheme presented in [6], we decompose Ψ into two functions $\Psi = \Psi_i + \Psi_e$ with Ψ_i convex and Ψ_e concave, and $\psi := \Psi' = \psi_i + \psi_e$, where

$$\Psi_i(u) := \frac{\theta}{2}\big[(1+u)\ln(1+u) + (1-u)\ln(1-u)\big], \qquad \psi_i(u) = \frac{\theta}{2}\ln\Big(\frac{1+u}{1-u}\Big),$$
$$\Psi_e(u) := \frac{\theta_c}{2}(1-u^2), \qquad \psi_e(u) = -\theta_c u.$$

We use the notation $i\sim$ and $e\sim$ to indicate implicit and explicit treatment of Ψ_i and Ψ_e in the time-stepping discretization, respectively, which leads to an unconditionally stable time discretization.

Let $T > 0$ denote a finite time, then the weak formulation of (1) demands finding $(u,\, w) \in L^\infty(0,T;\, H^1(\Omega)) \times L^2(0,T;\, H^1(\Omega))$ such that $u(x,0) = u_0(x)$ and

$$\langle u_t,\, v\rangle + (\nabla w,\, \nabla v) = 0, \qquad \forall v \in H^1(\Omega), \tag{2a}$$
$$(w,\, z) - (\psi,\, z) - \gamma(\nabla u,\, \nabla z) = 0, \qquad \forall z \in H^1(\Omega), \tag{2b}$$

where $\langle\cdot,\,\cdot\rangle$ denotes the duality pairing between $H^1(\Omega)$ and $H^{-1}(\Omega)$; and $(\cdot,\,\cdot)$ denotes the inner product in $L^2(\Omega)$.

The existence and uniqueness of this system for a class of Ψ has been shown in [1]. This system also has two interesting properties: Conservation of Mass and dissipative Free Energy $\mathcal{E}(u)$. Indeed, substituting $v \equiv 1$ in (2a) leads to $\int_\Omega u(t)\,dx = \int_\Omega u(0)\,dx$ and substituting $v = w$ and $z = u_t$ in (2) gives

$$\frac{d}{dt}\mathcal{E}(u(t)) = -\int_\Omega \gamma\,|\nabla w(t)|^2\,dx \quad \text{where} \quad \mathcal{E}(u) := \int_\Omega \frac{1}{2}|\nabla u|^2 + \Psi(u)\,dx.$$

2 Numerical Approximation

In order to formulate a finite element approximation of the problem (2), we focus on a polygon domain Ω, and construct a quasi-uniform family of triangulation $\mathbf{T}_h$ such that $\Omega = \bigcup_{\kappa\in\mathbf{T}_h}\kappa$ and $h := \max_{\kappa\in\mathbf{T}_h} h_\kappa$, where $h_\kappa := \operatorname{diam}(\kappa)$. We define the finite element space $S_h := \operatorname{span}(\{\varphi_r \in C(\Omega) \,:\, \varphi_r(x_k) = \delta_{rk}, \text{ for } r,k = 1,\dots,N_h\})$, where φ_r are the standard piecewise and continuous afine nodal basis functions and $\{x_r\}$ denotes the set of the vertices. Let $\{t_n = n\,\tau \,:\, n = 0,1,\dots,N, \text{ and } N\cdot\tau = T\}$ denote a discretization of time interval $[0,\,T]$ and τ the time-stepping size, and consider the first order approximation of u_t in time as $u_t(t_n) \approx [u(t_n) - u(t_{n-1})]/(t_n - t_{n-1})$. Our goal is to find $(\hat{u}^n, \hat{w}^n) \in S_h \times S_h$, where $\hat{u}^n := \hat{u}(t_n)$ and $\hat{w}^n := \hat{w}(t_n)$, such that for all $0 < n \le N$,

$$(\hat{u}^n - \hat{u}^{n-1},\, \hat{v})_h + \tau(\nabla\hat{w}^n,\, \nabla\hat{v}) = 0, \qquad \forall\,\hat{v} \in S_h \tag{3a}$$

$$(\hat{w}^n,\,\hat{z})_h - (\psi_i(\hat{u}^n) + \psi_e(\hat{u}^{n-1}),\,\hat{z})_h - \gamma(\nabla\hat{u}^n,\,\nabla\hat{z}) = 0, \qquad \forall\,\hat{z}\in S_h. \tag{3b}$$

where $(\cdot,\,\cdot)_h$ is the lumped discrete inner product defined as

$$(\hat{v},\hat{z})_h := \int_\Omega I_h(\hat{v}\,\hat{z})\,dx = \sum_{r=1}^{N_h} m_r\,\hat{v}(x_r)\,\hat{z}(x_r), \quad \forall\,\hat{v},\,\hat{z}\in S_h, \tag{4}$$

and I_h is the nodewise linear interpolation given by

$$I_h : C(\bar{\Omega}) \to S_h, \quad I_h v(x_r) = v(x_r) \;\text{ for }\; r = 1,\ldots,N_h, \tag{5}$$

$$m_r = (\varphi_r,\,\varphi_r)_h. \tag{6}$$

The proof of the existence of the discrete problem (3) follows from the convexity of the Ψ_i and lumped mass matrix approach considered in the discretization; The proof of the unconditionally time-stepping stability is similar to [6].

Theorem 1 *There exists a unique solution $(\hat{u}^n,\hat{w}^n)\in S_h\times S_h$ to the finite element problem (3).*

Proof The proof is a simple modification of the proof given in [6]. Let $(\hat{u}_1^n,\,\hat{w}_1^n)$ and $(\hat{u}_2^n,\,\hat{w}_2^n)$ be two solution of (3). By subtracting one solution from the other we get

$$(\hat{y}_u^n,\,\hat{v}) + \tau(\nabla\hat{y}_w^n,\,\nabla\hat{v}) = 0, \qquad \forall\,\hat{v}\in S_h, \tag{7a}$$

$$(\hat{y}_w^n,\,\hat{z}) - (\psi_i(\hat{u}_2^n) - \psi_i(\hat{u}_1^n),\hat{z}) - \gamma(\nabla\hat{y}_u^n,\,\nabla\hat{z}) = 0, \qquad \forall\,\hat{z}\in S_h. \tag{7b}$$

where $\hat{y}_u^n := \hat{u}_2^n - \hat{u}_1^n$ and $\hat{y}_w^n := \hat{w}_2^n - \hat{w}_1^n$. Substituting $\hat{v}$ and $\hat{z}$ into (7) with $\hat{y}_w^n$ and $\hat{y}_u^n$, respectively, leads to

$$\tau|\hat{y}_w^n|_1^2 + \gamma|\hat{y}_u^n|_1^2 = \big(\psi_i(\hat{u}_1^n) - \psi_i(\hat{u}_2^n)_h,\,\hat{y}_u^n\big),$$

where $|\cdot|_1$ denotes the seminorm of $H^1(\Omega)$. Applying the mean value theorem to ψ_i gives

$$\big(\psi_i(s_1) - \psi_i(s_2)\big)(s_2 - s_1) = -\psi_i'(c)(s_2 - s_1)^2,$$

for every $s_1,\,s_2\in(-1,1)$ and c between s_1 and s_2. Based on the convexity of ψ_i we get $0\le\psi_i'(s)$ for $s\in(-1,1)$, which implies

$$\big(\psi_i(\hat{u}_1^n) - \psi_i(\hat{u}_2^n),\,\hat{y}_u^n\big)_h \le 0,$$

and accordingly $\tau\,|\hat{y}_w^n|_1^2 + \gamma\,|\hat{y}_u^n|_1^2 \le 0$. Moreover, since $(\hat{y}_u^n,1)_h = 0$, the Poincaré inequality implies that $\|\hat{y}_u^n\| = 0$. To show the uniqueness of $\hat{w}^n$ it suffices to set $\hat{z}$ equal to $\hat{y}_w^n$ in (7b) and get $\|\hat{y}_w^n\| = 0$. This concludes the proof of uniqueness. □

3 Newton's Method

Our objective is to solve the nonlinear system (3) using Newton's method. Since the nonlinearity is associated with the potential function Ψ, for every Newton's iteration j and time step n, we set

$$\hat{u}_j^n = \hat{u}_{j-1}^n - \delta\hat{u}_j^n. \tag{8}$$

Substituting $(\hat{u}^n,\ \hat{w}^n)$ with $(\hat{u}_j^n,\ \hat{w}_j^n)$ in (3) and using the linearization

$$\psi_i(\hat{u}_j^n) \approx \psi_i(\hat{u}_{j-1}^n) - \psi_i'(\hat{u}_{j-1}^n)\,\delta\hat{u}_j^n, \tag{9}$$

the system of equation in (3) leads to

$$(\delta\hat{u}_j^n,\ \hat{v})_h - \tau\,(\nabla\hat{w}_j^n,\ \nabla\hat{v}) = \phi_1(\hat{v}), \qquad \forall\,\hat{v}\in S_h, \tag{10a}$$

$$\big(\psi_i'(\hat{u}_{j-1}^n)\,\delta\hat{u}_j^n,\ \hat{z}\big)_h + \gamma\,(\nabla\delta\hat{u}_j^n,\ \nabla\hat{z}) + (\hat{w}_j^n,\ \hat{z})_h = \phi_2(\hat{z}), \qquad \forall\,\hat{z}\in S_h, \tag{10b}$$

where

$$\phi_1(\hat{v}) := (\hat{u}_{j-1}^n - \hat{u}^{n-1},\ \hat{v})_h, \tag{11a}$$

$$\phi_2(\hat{z}) := \big(\psi_i(\hat{u}_{j-1}^n) + \psi_e(\hat{u}^{n-1}),\ \hat{z}\big)_h + \gamma\,(\nabla\hat{u}_{j-1}^n,\ \nabla\hat{z}). \tag{11b}$$

Let $\mathbf{u}_j^n$, $\mathbf{w}_j^n$ and $\boldsymbol{\delta}\mathbf{u}_j^n$ in $\mathbb{R}^{N_h}$ denote the vectors composed of the values of $\hat{u}_j^n$, $\hat{w}_j^n$ and $\delta\hat{u}_j^n$ evaluated at every vertex x_r, that is $[\mathbf{u}_j^n]_r = \hat{u}_j^n(x_r)$, $[\mathbf{w}_j^n]_r = \hat{w}_j^n(x_r)$ and $[\boldsymbol{\delta}\mathbf{u}_j^n]_r = \delta\hat{u}_j^n(x_r)$. In addition, let $[M]_{r,k} := (\varphi_r, \varphi_k)_h$, $[K]_{r,k} := (\nabla\varphi_r,\ \nabla\varphi_k)$ and

$$[J_{j-1}]_{r,k} := \Big(\psi_i'\big(\sum_{l=1}^{N_h}[\mathbf{u}_{j-1}^n]_l\varphi_l\big)\varphi_r\ ,\ \varphi_k\Big)_h, \qquad \tilde{K} := K,$$

$$[\mathbf{q}_{j-1}]_r := \Big(\psi_i\big(\sum_{l=1}^{N_h}[\mathbf{u}_{j-1}^n]_l\varphi_l\big), \varphi_r\Big)_h, \qquad [\mathbf{p}]_r := \Big(\psi_e\big(\sum_{l=1}^{N_h}[\mathbf{u}^{n-1}]_l\varphi_l\big), \varphi_r\Big)_h.$$

Then, the discrete representation of (10) yields

$$M\,\boldsymbol{\delta}\mathbf{u}_j^n - \tau\,K\,\mathbf{w}_j^n = \mathbf{f}_{j-1} \tag{12a}$$

$$M^T\,\mathbf{w}_j^n + (J_{j-1} + \gamma\,\tilde{K})\,\boldsymbol{\delta}\mathbf{u}_j^n = \mathbf{g}_{j-1}, \tag{12b}$$

$$\mathbf{u}_j^n = \mathbf{u}_{j-1}^n - \boldsymbol{\delta}\mathbf{u}_j^n. \tag{12c}$$

where $\mathbf{f}_{j-1} = M(\mathbf{u}_{j-1}^n - \mathbf{u}^{n-1})$ and $\mathbf{g}_{j-1} = \mathbf{q}_{j-1} + \mathbf{p} + \gamma\,\tilde{K}\,\mathbf{u}_{j-1}^n$.

Let $\Omega = (0,1)^2$ and $\mathbf{T}_h$ be a uniform triangulation with 45-degrees triangles where $h = 1/32$, $\tau = 0.01$, $\gamma = h^2$ with a random initial condition $\mathbf{u}^0$. Fig. 1 illustrates the numerical solution at six time instances. The Newton's method is stopped when $\|\boldsymbol{\delta}\mathbf{u}^n\|_{\ell_\infty} \le 10^{-10}$. The color map that varies from blue (dark) to yellow (light) depicts values of $\mathbf{u}^n(x_r)$ close to -1^+ and $+1^-$, respectively.

4 Preconditioned Iterative Solver

We consider solving (12) simultaneously to find $\mathbf{w}_j^n$ and $\boldsymbol{\delta}\mathbf{u}_j^n$ as a solution to

$$A\,\mathbf{x} = \begin{bmatrix} -\tau K & M \\ M^T & J_{j-1} + \gamma \tilde{K} \end{bmatrix} \begin{bmatrix} \mathbf{w}_j^n \\ \boldsymbol{\delta}\mathbf{u}_j^n \end{bmatrix} = \begin{bmatrix} \mathbf{f}_{j-1} \\ \mathbf{g}_{j-1} \end{bmatrix} = \mathbf{b}. \tag{13}$$

Since the associated matrix is symmetric, we can use MinRes algorithm to find $(\mathbf{w}_j^n,\, \boldsymbol{\delta}\mathbf{u}_j^n)$ at each Newton's iteration. We now propose a preconditioner based on the Schur complememt of the first block of (13) given by

$$B_1 = \begin{bmatrix} -M(J_{j-1} + \gamma\tilde{K})^{-1}M^T - \tau K & 0 \\ 0 & J_{j-1} + \gamma\tilde{K} \end{bmatrix}. \tag{14}$$

In what follows, we investigate the performance of the solver based on the proposed

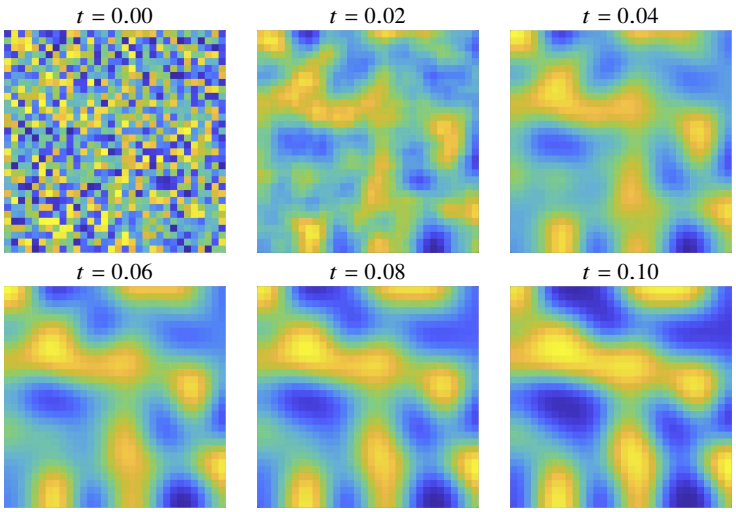

Fig. 1: numerical solution of (12) at $t = 0,\ 0.02,\ 0.04,\ 0.06,\ 0.08,$ and 0.1 for $\Omega = (0,1)^2$, $h = 1/32$, $\tau = 0.01$, $\gamma = h^2$ and a random initial condition $\mathbf{u}^0$.

$P_1\,\mathbf{x} = B_1^{-1}\,A\,\mathbf{x} = B_1^{-1}\,\mathbf{b}$. Note that, since the lumped inner products is utilized, M and J_{j-1} are diagonal matrices. See also [4] for other class of preconditioners.

Table 1 demonstrates the behavior of the preconditioned system P_1. As listed, the preconditioned system requires six Newton's iterations for the first, and four iterations for the second time step. The table includes number of MinRes iterations that reduce the preconditioned residue by a 10^{-6} factor. As time goes on, the solution becomes more regular (see Fig. 1) and demands less number of Newton's iterations. Note that A is symmetric and B_1 is symmetric positive definite. We note that, without

utilizing the preconditioner, the solver may not converge or the convergence is much slower. In Table 2 we consider $P_2\,\mathbf{x} = B_2^{-1}\,A\,\mathbf{x} = B_2^{-1}\,\mathbf{b}$ where B_2^{-1} is a BPX [3] type

n	j	$\|\delta\mathbf{u}_j^n\|_\infty$	relres	gmres itrs
1	1	9.342e-01	6.272e-07	25
1	2	4.144e-01	6.748e-07	27
1	3	1.548e-02	8.128e-07	26
1	4	3.020e-05	8.109e-07	26
1	5	1.133e-10	8.109e-07	26
1	6	2.112e-16	8.109e-07	26
2	1	2.651e-01	7.713e-07	27
2	2	4.494e-03	6.102e-07	28
2	3	3.427e-06	6.140e-07	28
2	4	2.031e-12	6.140e-07	28

Table 1: Results of solving (13) using preconditioned system P_1 with lumped matrices M and J_{j-1} for $h = 1/32$, $\tau = 0.01$, $\gamma = h^2$ and a random initial condition $\mathbf{u}^0$.

preconditioner. The BPX method we consider here follows the strategy in [8, 7] that deals with rational functions of Sobolev norms; this work was motivated from the BPX introduced in [2] that deals with sum of Sobolev norms of the same sign. The multilevel preconditioner is defined as $B_2^{-1} = \mathrm{diag}\{D_1, D_2\}$ with

$$D_1 = -\sum_k R_k^T \left[\left(\mathrm{diag}_k \left\{ R_k M^{-1} (J_{j-1} + \gamma \tilde{K}) M^{-1} R_k^T \right\} \right)^{-1} + \mathrm{diag}_k \{ R_k \tau K R_k^T \} \right]^{-1} R_k,$$

$$D_2 = \sum_k R_k^T \left(\mathrm{diag}_k \left\{ R_k (J_{j-1} + \gamma \tilde{K}) R_k^T \right\} \right)^{-1} R_k,$$

where D_1 and D_2 are diagonal matrices, R_k^T is the prolongation operator from k-level to fine level and $\mathrm{diag}_k\{C_k\}$ is the diagonal of the matrix C_k defined on the k-level.

As listed in Table 2, the number of iterations using the inexact BPX preconditioner (B_2^{-1}) is comparable with the exact preconditioner B_1^{-1}. See also [4] where the Schur complememt of the second block is considered. In Table 3, we test the behavior of preconditioned systems P_1 and P_2 as we vary τ for fixed $\gamma = h^2 = (1/16)^2$. As listed, the number of MinRes iterations for P_1 and P_2 is smaller for larger time-stepping size τ. This is not surprising, since, as we increase τ, the Schur complement $M\,(J_{j-1} + \gamma\,\tilde{K})^{-1}\,M^T + \tau\,K$ becomes more positive definite. The result of changing $\gamma = h^2$ for fixed $\tau = 0.01$ is listed in Table 4. As depicted in the table, the number of MinRes iterations of both P_1 and P_2 is very robust with respect to mesh size h. We note that the condition $\gamma = O(h^2)$ is a reasonable choice since the size of the transition layer of u from -1 to 1 is $O(\sqrt{\gamma})$. Note that, we use a random initial condition $\mathbf{u}^0$ and utilize the lumped matrices[1] when defining M and J_{j-1}.

[1] This is a consequence of using the inner product $(\cdot,\ \cdot)_h$ as defined in (4)

n	j	$\|\delta \mathbf{u}_j^n\|_\infty$	relres	gmres itrs
1	1	9.342e-01	7.115e-07	50
1	2	4.144e-01	7.393e-07	58
1	3	1.548e-02	7.555e-07	57
1	4	3.020e-05	7.575e-07	51
1	5	1.132e-10	7.575e-07	57
1	6	2.202e-16	7.575e-07	57
2	1	2.651e-01	7.712e-07	59
2	2	4.494e-03	8.443e-07	59
2	3	3.427e-06	8.430e-07	59
2	4	2.025e-12	8.430e-07	59

Table 2: Results of solving (13) using preconditioned system P_2 with lumped matrices M and J_{j-1} for $h = 1/32$, $\tau = 0.01$, $\gamma = h^2$ and a random initial condition $\mathbf{u}^0$.

τ	n	Exact P_1		Additive multigrid P_2	
		Newton stp	solver itr.	Newton stp	solver itr.
0.1	1	6	18	6	32
	2	4	19	4	34
	3	4	19	4	34
	4	5	19	5	34
0.01	1	5	24	5	51
	2	4	26	4	53
	3	4	26	4	53
	4	4	26	4	53
0.001	1	5	26	5	87
	2	4	27	4	90
	3	4	27	4	90
	4	4	27	4	90

Table 3: Results of varying τ for fixed $\gamma = h^2 = (1/16)^2$. Number of solver iterations (solver itr.) reported in the table are the average over the Newton's iterations at every time step n. Preconditioned systems P_1 and P_2 are constructed using lumped matrices M and J_{j-1} and the initial conditions for all is a fixed random $\mathbf{u}^0$.

5 Conclusions

Our main contribution is the development of a robust multilevel PBX-type preconditioner for a finite element approximation of the Cahn-Hilliard problem. The numerical results provided demonstrate the robustness of the preconditioned systems with respect to mesh size and time steps.

References

1. Miranville A. and S Zelik. Exponential attractors for the Cahn-Hilliard equation with dynamic boundary conditions. *Math. Methods Appl. Sci.*, 28(6):709–745, 1992.

h	n	Exact P_1		Additive multigrid P_2	
		Newton stp	solver itr.	Newton stp	solver itr.
1/16	1	5	24	5	51
	2	4	26	4	53
	3	4	26	4	53
	4	4	26	4	53
1/32	1	6	26	6	56
	2	4	28	4	59
	3	4	29	4	60
	4	4	28	4	60
1/64	1	6	27	6	58
	2	4	29	4	61
	3	5	30	5	62
	4	5	30	5	62

Table 4: Results of varying $\gamma = h^2$ for fixed $\tau = 0.01$. Number of solver iterations (solver itr.) reported in the table are the average over the Newton's iterations at every time step n. Preconditioned systems P_1 and P_2 are constructed using lumped matrices M and J_{j-1} and the initial conditions for all is a fixed random $\mathbf{u}^0$.

2. James H. Bramble, Joseph E. Pasciak, and Panayot S. Vassilevski. Computational scales of Sobolev norms with application to preconditioning. *Math. Comp.*, 69(230):463–480, 2000.
3. James H. Bramble, Joseph E. Pasciak, and Jinchao Xu. Parallel multilevel preconditioners. *Math. Comp.*, 55(191):1–22, 1990.
4. Susanne C Brenner, Amanda E Diegel, and Li-Yeng Sung. A robust solver for a mixed finite element method for the Cahn–Hilliard equation. *Journal of Scientific Computing*, 77(2):1234–1249, 2018.
5. John W Cahn and John E Hilliard. Free energy of a nonuniform system. i. interfacial free energy. *The Journal of Chemical Physics*, 28(2):258–267, 1958.
6. M. I. M. Copetti and C. M. Elliott. Numerical analysis of the Cahn-Hilliard equation with a logarithmic free energy. *Numer. Math.*, 63(1):39–65, 1992.
7. Etereldes Gonçalves and Marcus Sarkis. Analysis of robust parameter-free multilevel methods for Neumann boundary control problems. *Comput. Methods Appl. Math.*, 13(2):207–235, 2013.
8. Etereldes Gonçalves and Marcus Sarkis. Robust parameter-free multilevel methods for Neumann boundary control problems. In *Domain decomposition methods in science and engineering XX*, volume 91 of *Lect. Notes Comput. Sci. Eng.*, pages 111–118. Springer, Heidelberg, 2013.