Multigrid Methods for the Biharmonic Problem with Cahn-Hilliard Boundary Conditions

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1 Introduction

Let $\Omega \subset \mathbb{R}^2$ be a bounded polygonal domain, $V = \{v \in H^2(\Omega) : \partial v/\partial n = 0 \text{ on } \partial\Omega\}$ and $f \in L_2(\Omega)$. In this paper we consider multigrid methods for the following biharmonic problem: Find $u \in V$ such that

$$\int_\Omega \nabla^2 u : \nabla^2 v \, dx = \int_\Omega f v \, dx \qquad \forall v \in V, \tag{1}$$

where $\nabla^2 w : \nabla^2 v = \sum_{i,j=1}^2 w_{x_i x_j} v_{x_i x_j}$ is the inner product of the Hessian matrices of w and v. Under the (assumed) compatibility condition,

$$\int_\Omega f \, dx = 0, \tag{2}$$

the biharmonic problem (1) is solvable and the solution is unique up to an additive constant. Furthermore we have an elliptic regularity estimate

$$\|\hat{u}\|_{H^{2+\alpha}(\Omega)} \le C \|f\|_{L_2(\Omega)} \tag{3}$$

for the solution $\hat{u}$ of (1) that satisfies $\int_\Omega \hat{u} \, dx = 0$. Note that, unlike the biharmonic problem with the boundary conditions of clamped plates, the index of elliptic regularity α in (3), which is determined by the angles of Ω, can be close to 0 even if Ω is convex (cf. [2]).

The essential boundary condition $\partial u/\partial n = 0$ and the natural boundary condition $\partial(\Delta u)/\partial n = 0$ satisfied by the solution u of (1) appear in the Cahn-Hilliard model for phase separation phenomena (cf. [8]). In particular, the boundary value problem (1) appears when the Cahn-Hilliard equation is discretized in time by an implicit method and the resulting nonlinear fourth order elliptic boundary value problem is solved by an Newton iteration.

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We will describe a C^0 interior penalty method for (1) in Sect. 2 and introduce in Sect. 3 multigrid methods that are based on a new smoother. The convergence properties of the multigrid methods are briefly discussed in Sect. 4, followed by numerical results in Sect. 5.

2 A Quadratic C^0 Interior Penalty Method

C^0 interior penalty methods (cf. [6, 9]) are discontinuous Galerkin methods for fourth order problems. Let $\mathscr{T}_h$ be a simplicial triangulation of Ω, $V_h \subset H^1(\Omega)$ be the associated P_2 Lagrange finite element space (cf. [5]), and $\hat{V}_h$ be the subspace of V_h consisting of functions with zero mean, i.e., $v \in V_h$ belongs to $\hat{V}_h$ if and only if $\int_\Omega v\,dx = 0$. The quadratic C^0 interior penalty method for (1) is to find $\hat{u}_h \in \hat{V}_h$ such that

$$a_h(\hat{u}_h, v) = \int_\Omega f v\,dx \qquad \forall\, v \in \hat{V}_h, \tag{4}$$

where

$$\begin{aligned} a_h(w,v) = &\sum_{T\in\mathscr{T}_h}\int_T \nabla^2 w : \nabla^2 v\,dx + \sum_{e\in\mathscr{E}_h}\int_e \left\{\!\!\left\{ \frac{\partial^2 w}{\partial n^2} \right\}\!\!\right\} \left[\!\!\left[\frac{\partial v}{\partial n} \right]\!\!\right] ds \\ &+ \sum_{e\in\mathscr{E}_h}\int_e \left\{\!\!\left\{ \frac{\partial^2 v}{\partial n^2} \right\}\!\!\right\} \left[\!\!\left[\frac{\partial w}{\partial n} \right]\!\!\right] ds + \sum_{e\in\mathscr{E}_h} \frac{\sigma}{|e|}\int_e \left[\!\!\left[\frac{\partial w}{\partial n} \right]\!\!\right] \left[\!\!\left[\frac{\partial v}{\partial n} \right]\!\!\right] ds. \end{aligned} \tag{5}$$

Here $\mathscr{E}_h$ is the set of the edges in $\mathscr{T}_h$, $\{\!\{\partial^2 v/\partial n^2\}\!\}$ (resp. $[\![\partial v/\partial n]\!]$) is the average of the second normal derivative of v (resp. the jump of the first normal derivative of v) across an edge, $|e|$ is the length of the edge e, and $\sigma > 0$ is a penalty parameter.

The quadratic C^0 interior penalty method is consistent. It is also stable if σ is sufficiently large, which is assumed to be the case. (The magnitude of σ is related to certain inverse estimates. It can be taken to be 5 in practice.) It can be shown (cf. [3]) that the solution $\hat{u}_h$ of (4) satisfies the following error estimate:

$$\|\hat{u} - \hat{u}_h\|_h \le Ch^\alpha \|f\|_{L_2(\Omega)}, \tag{6}$$

where $\hat{u}$ is the zero mean solution of (1), α is the index of elliptic regularity in (3), and the norm $\|\cdot\|_h$ is given by

$$\|v\|_h^2 = \sum_{T\in\mathscr{T}_h} |v|_{H^2(T)}^2 + \sum_{e\in\mathscr{E}_h} |e|^{-1} \|[\![\partial v/\partial n]\!]\|_{L_2(e)}^2.$$

C^0 interior penalty methods have certain advantages over other finite element methods for fourth order problems. They are simpler than conforming methods which require C^1 elements. They come in a natural hierarchy that can capture smooth solutions efficiently, which is not the case for classical nonconforming methods. Unlike mixed methods they preserve the positive definiteness of the continuous problem and are easier to develop for more complicated problems (cf. [9]).

Another significant advantage of C^0 interior penalty methods comes from the fact that the underlying finite element spaces are standard spaces for second order problems. (Note that the essential boundary condition for (1) is only enforced weakly in (4) and the finite element space V_h does not involve any boundary condition.) Therefore multigrid solves for second order problems can be easily implemented as a preconditioner. By using such a preconditioner in the smoothing steps of multigrid algorithms for fourth order problems, the performance of the smoother and hence the overall performance of the multigrid algorithms can be significantly improved. This approach was carried out in [7] for the biharmonic problem with the boundary conditions of clamped plates. Below we will use this approach to develop multigrid methods for (4).

3 Multigrid Methods

Let $\mathcal{T}_k$ $(k = 0, 1, \cdots)$ be a sequence of simplicial triangulations obtained from the initial triangulation $\mathcal{T}_0$ by uniform refinement. We will use V_k (resp. $a_k(\cdot,\cdot)$) to denote the finite element space (resp. the bilinear form for the C^0 interior penalty method) associated with $\mathcal{T}_k$.

Let V_k' be the dual space of V_k and $\hat{V}_k = \{v \in V_k : \int_\Omega v\,dx = 0\}$ be the zero-mean subspace of V_k. We can identify $\hat{V}_k'$ with the subspace of V_k' whose members annihilate the constant functions, i.e., $\hat{V}_k' = \{\gamma \in V_k' : \langle \gamma, 1\rangle = 0\}$, where $\langle\cdot,\cdot\rangle$ is the canonical bilinear form between a vector space and its dual.

Let the operator $A_k : V_k \longrightarrow V_k'$ be defined by $\langle A_k v, w\rangle = a_k(v, w)$ for all $v, w \in V_k$. We can then rewrite the discrete problem (4) as $A_k\hat{u}_k = \phi_k$, where $\hat{u}_k \in \hat{V}_k$ and $\phi_k \in \hat{V}_k'$ satisfies $\langle \phi_k, v\rangle = \int_\Omega f v\,dx$ for all $v \in V_k$. Below we will develop multigrid algorithms for equations of the form

$$A_k z = \psi \tag{7}$$

where $z \in \hat{V}_k$ and $\psi \in \hat{V}_k'$.

There are two ingredients in the design of multigrid algorithms. First of all, we need intergrid transfer operators to move data between consecutive levels. Since the finite element spaces are nested, we can take the coarse-to-fine operator $I_{k-1}^k : V_{k-1} \longrightarrow V_k$ to be the natural injection and the fine-to-coarse operator $I_k^{k-1} : V_k' \longrightarrow V_{k-1}'$ to be the transpose of I_{k-1}^k with respect to the canonical bilinear forms, i.e., $\langle I_k^{k-1}\gamma, v\rangle = \langle \gamma, I_{k-1}^k v\rangle$ for all $\gamma \in V_k'$, $v \in V_{k-1}$. Note that I_{k-1}^k maps $\hat{V}_{k-1}$ into $\hat{V}_k$ and consequently I_k^{k-1} maps $\hat{V}_k'$ into $\hat{V}_{k-1}'$.

The second ingredient is a good smoother that can damp out the highly oscillatory part of the error of an approximate solution so that the remaining part of the error can be captured accurately on a coarser grid. Here we take advantage of the fact that the P_2 Lagrange finite element space is a standard space for second order problems to incorporate a multigrid Poisson solve in the smoother. Let $L_k : \hat{V}_k \longrightarrow \hat{V}_k'$ be the discrete Laplace operator defined by

$$\langle L_k v, w\rangle = \int_\Omega \nabla v \cdot \nabla w\,dx \qquad \forall v, w \in \hat{V}_k.$$

We take $S_k^{-1}:\hat{V}_k' \longrightarrow \hat{V}_k$ to be an approximate inverse of L_k obtained from a multigrid Poisson solve such that

$$\langle S_k v, v\rangle \approx |v|^2_{H^1(\Omega)} \qquad \forall\, v \in \hat{V}_k. \tag{8}$$

The smoothing step in our multigrid algorithms for (7) is then given by

$$z_{\text{new}} = z_{\text{old}} + \lambda_k S_k^{-1}(\psi - A_k z_{\text{old}}), \tag{9}$$

where λ_k is a damping factor chosen so that the spectral radius $\rho(\lambda_k S_k^{-1} A_k)$ is <2. It follows from (8) and standard inverse estimates (cf. [5]) that we can take $\lambda_k = Ch_k^2$. Note that the computational cost of (9) is proportional to the dimension of $\hat{V}_k$, which implies that the overall computational costs of the multigrid algorithms in Sects. 3.1 and 3.2 are also proportional to the dimension of $\hat{V}_k$.

We can now describe the V-cycle and W-cycle algorithms (cf. [10]) in terms of the intergrid transfer operators and the smoothing scheme.

3.1 V-Cycle Algorithm

The V-cycle algorithm computes an approximate solution $MG_V(k,\psi,z_0,m)$ of (7) with initial guess $z_0 \in \hat{V}_k$ and m pre-smoothing and m post-smoothing steps. For $k=0$, we take $MG_V(0,\psi,z_0,m)$ to be the output of a direct solve. For $k \geq 1$, we compute $MG_V(k,\psi,z_0,m)$ recursively in three steps.

Pre-smoothing For $1 \leq \ell \leq m$, compute z_ℓ recursively by

$$z_\ell = z_{\ell-1} + \lambda_k S_k^{-1}(\psi - A_k z_{\ell-1}).$$

Coarse Grid Correction Compute

$$z_{m+1} = z_m + I_{k-1}^k MG_V(k-1,\rho_{k-1},0,m),$$

where $\rho_{k-1} = I_k^{k-1}(\psi - A_k z_m) \in \hat{V}_{k-1}'$ is the transferred residual of z_m.

Post-smoothing For $m+2 \leq \ell \leq 2m+1$, compute z_ℓ recursively by

$$z_\ell = z_{\ell-1} + \lambda_k S_k^{-1}(\psi - A_k z_{\ell-1}).$$

The final output is $MG_V(k,\psi,z_0,m) = z_{2m+1}$.

3.2 W-Cycle Algorithm

The W-cycle algorithm computes an approximate solution $MG_W(k,\psi,z_0,m)$ of (7) with initial guess $z_0 \in \hat{V}_k$ and m pre-smoothing and m post-smoothing steps. The only difference between the V-cycle algorithm and the W-cycle algorithm is in the coarse grid correction step, where the coarse grid algorithm is applied twice to the coarse grid residual equation. More precisely, we have

$$\begin{aligned} z_{m+\frac{1}{2}} &= MG_W(k-1,\rho_{k-1},0,m),\\ z_{m+1} &= z_m + MG_W(k-1,\rho_{k-1},z_{m+\frac{1}{2}},m). \end{aligned}$$

Remark 1. For simplicity we have described the multigrid algorithms in terms of the space $\hat{V}_k$ where the bilinear form $a_k(\cdot,\cdot)$ is nonsingular. But the multigrid Poisson solve S_k^{-1} (and hence the V-cycle and W-cycle algorithms) can be implemented on V_k for $k \geq 1$. The implementation of multigrid algorithms for the singular Neumann problem is discussed for example in [1].

4 Convergence Properties

Let $z_0 \in \hat{V}_k$ be the initial guess and $z_\dagger \in \hat{V}_k$ be the output of the V-cycle or W-cycle algorithm for (7). Numerical results indicate that

$$\|z - z_\dagger\|_{a_h} \leq Cm^{-\alpha}\|z - z_0\|_{a_h}, \tag{10}$$

where α is the index of elliptic regularity in (3) and $\|\cdot\|_{a_h} = \sqrt{a_h(\cdot,\cdot)}$ is the energy norm, provided that the number of smoothing steps $m \geq m_*$. Here m_* is a sufficiently large positive integer independent of k. In particular the multigrid algorithms are contractions for sufficiently large m and the contraction numbers are bounded away from 1 uniformly. A similar estimate was obtained in [7] for the boundary conditions of clamped plates. The derivation of (10) for the Cahn-Hilliard boundary conditions will be carried out in [4] where general fourth order problems are considered.

A significant benefit of including a multigrid Poisson solve in the smoothing step (9) is that the resulting smoothing property is similar to that for second order problems (cf. [7]) so that the contraction number estimate (10) is also similar to that for second order problems. Indeed, because of the estimate (8), we can derive a smoothing property for (9) with respect to a family of mesh dependent norms $|||\cdot|||_{s,k}$ such that $|||\cdot|||_{0,k} \approx |\cdot|_{H^1(\Omega)}$ and $|||\cdot|||_{1,k} \approx |\cdot|_{H^2(\Omega)}$ on the space $\hat{V}_k$. Note that the smoothing properties of standard smoothers for second order problems are described in terms of mesh dependent norms $|||\cdot|||_{s,k}$ such that $|||\cdot|||_{0,k} \approx \|\cdot\|_{L_2(\Omega)}$ and $|||\cdot|||_{1,k} \approx |\cdot|_{H^1(\Omega)}$ on the finite element spaces. The good performance of the smoothing step (9) is due to the similarity between the Hilbert scales $[H^1(\Omega), H^2(\Omega)]$ and $[L_2(\Omega), H^1(\Omega)]$.

If we use a standard smoother such as the Richardson relaxation in a multigrid algorithm for (7), then the smoothing property will be determined by the Hilbert scale $[L_2(\Omega), H^2(\Omega)]$. In this case the estimate (10) will be replaced by the estimate

$$\|z - z_\dagger\|_{a_h} \leq Cm^{-\alpha/2}\|z - z_0\|_{a_h}, \tag{11}$$

which means that the effect of 100 smoothing steps without the preconditioner is roughly equivalent to the effect of 10 smoothing steps with the preconditioner. As far as we know, all existing multigrid methods for fourth order problems (except those in [6]) use standard smoothers and their convergence is governed by (11).

5 Numerical Results

The numerical experiments were performed on sienna@IMA (Intel P4, 3.4 GHz CPU, 2 G memory) at the Institute for Mathematics and its Applications. In the numerical experiments we take $\sigma = 5$ and the preconditioner to be a V-cycle Poisson

solve with one pre-smoothing step and one post-smoothing step. (Other multigrid Poisson solves can also be used, but the $V(1,1)$ solve appears to be the most efficient.) The contraction numbers for the V-cycle and W-cycle algorithms on the unit square (with two elements in the initial mesh) are reported in Tables 1 and 2. It is observed that the V-cycle (resp. W-cycle) algorithm is a contraction for $m \geq 4$ (resp. $m \geq 2$).

Table 1. Contraction numbers for the V-cycle algorithm on the unit square.

k \ m	4	5	6	7	8	9	10	11	12	13
1	0.212	0.126	0.0813	0.0594	0.0442	0.0332	0.0252	0.0192	0.0147	0.0114
2	0.329	0.223	0.190	0.164	0.142	0.124	0.109	0.0967	0.0861	0.0771
3	0.412	0.342	0.308	0.279	0.255	0.234	0.217	0.203	0.190	0.179
4	0.479	0.420	0.386	0.357	0.334	0.314	0.296	0.282	0.266	0.257
5	0.537	0.467	0.434	0.408	0.386	0.367	0.351	0.336	0.324	0.312
6	0.578	0.494	0.462	0.436	0.415	0.396	0.380	0.366	0.353	0.341
7	0.619	0.503	0.472	0.446	0.425	0.406	0.391	0.376	0.364	0.351

Table 2. Contraction numbers for the W-cycle algorithm on the unit square.

k \ m	2	3	4	5	6	7	8	9	10	11
1	0.661	0.368	0.212	0.126	0.0813	0.0594	0.0442	0.0332	0.0252	0.0192
2	0.483	0.360	0.291	0.241	0.203	0.172	0.148	0.128	0.112	0.0983
3	0.475	0.375	0.335	0.282	0.263	0.229	0.215	0.195	0.182	0.171
4	0.455	0.383	0.335	0.308	0.287	0.270	0.256	0.244	0.233	0.223
5	0.456	0.384	0.344	0.315	0.297	0.279	0.267	0.255	0.245	0.237
6	0.455	0.384	0.344	0.316	0.297	0.280	0.268	0.256	0.248	0.239
7	0.455	0.384	0.344	0.317	0.297	0.281	0.269	0.258	0.248	0.240

For comparison we report in Table 3 the contraction numbers for the V-cycle algorithm that does not use a preconditioner in the smoothing steps. The smoothing step in this algorithm is the standard Richardson relaxation scheme.

We have also carried out numerical experiments for the L-shaped domain with vertices $(0,0)$, $(1,0)$, $(1,1)$, $(-1,1)$, $(-1,-1)$ and $(0,-1)$. The initial mesh consists of six isosceles triangles sharing $(0,0)$ as a common vertex. The contraction numbers for the W-cycle algorithm with/without the preconditioner are presented in Tables 4 and 5.

We note that the contraction numbers in Table 1 (resp. Table 4) for m smoothing steps are comparable to the contraction numbers in Table 3 (resp. Tables 5) for m^2 smoothing steps.

Table 3. Contraction numbers for the V-cycle algorithm without a preconditioner on the unit square.

k \ m	21	22	23	24	25	26	27	28	29	30
1	0.428	0.410	0.392	0.376	0.361	0.346	0.332	0.320	0.307	0.296
2	0.646	0.614	0.583	0.555	0.529	0.504	0.481	0.459	0.439	0.420
3	0.770	0.728	0.690	0.654	0.621	0.591	0.562	0.535	0.510	0.487
4	0.844	0.797	0.753	0.713	0.676	0.641	0.609	0.579	0.551	0.525
5	0.895	0.843	0.795	0.752	0.711	0.674	0.639	0.607	0.577	0.548
6	0.931	0.876	0.826	0.780	0.737	0.697	0.661	0.627	0.595	0.565
7	0.960	0.902	0.849	0.801	0.757	0.715	0.677	0.642	0.609	0.578

Table 4. Contraction numbers for the W-cycle algorithm with a preconditioner on the L-shaped domain.

k \ m	3	5	7	9	11	13	15	17	19	21	23
1	0.319	0.187	0.125	0.105	0.0913	0.0798	0.0699	0.0614	0.0540	0.0476	0.0420
2	0.383	0.273	0.206	0.161	0.139	0.132	0.125	0.119	0.113	0.108	0.103
3	0.390	0.302	0.238	0.208	0.182	0.163	0.152	0.148	0.144	0.141	0.137
4	0.386	0.309	0.271	0.245	0.224	0.208	0.193	0.181	0.170	0.161	0.153
5	0.384	0.315	0.279	0.255	0.237	0.222	0.209	0.198	0.189	0.180	0.172
6	0.384	0.316	0.281	0.257	0.240	0.226	0.213	0.203	0.193	0.185	0.177
7	0.387	0.317	0.281	0.258	0.240	0.226	0.214	0.203	0.194	0.186	0.178

Table 5. Contraction numbers for the W-cycle algorithm without a preconditioner on the L-shaped domain.

k \ m	5	7	9	11	13	15	17	19	21	23
1	0.943	0.788	0.680	0.600	0.537	0.486	0.443	0.407	0.375	0.347
2	0.790	0.585	0.505	0.459	0.426	0.394	0.375	0.358	0.342	0.328
3	0.666	0.512	0.469	0.456	0.434	0.416	0.400	0.386	0.373	0.362
4	0.580	0.519	0.484	0.454	0.434	0.418	0.405	0.394	0.385	0.376
5	0.581	0.527	0.491	0.465	0.444	0.427	0.414	0.402	0.392	0.384
6	0.587	0.531	0.494	0.467	0.446	0.429	0.415	0.404	0.394	0.386
7	0.587	0.530	0.493	0.467	0.446	0.429	0.415	0.404	0.394	0.386

Finally we compare the computational cost between the preconditioned schemes and the un-preconditioned schemes. On the unit square, the contraction numbers for the preconditioned V-cycle algorithm with $m = 4$ (cf. Table 1) are about the same as the contraction numbers for the un-preconditioned V-cycle algorithm with $m = 29$ (cf. Table 3). For $k = 7$, the former takes 1.4×10^8 floating point operations and 0.55 s while the latter takes 3.2×10^8 floating point operations and 1.2 s.

On the L-shaped domain, the contraction numbers for the preconditioned W-cycle algorithm with $m = 3$ (cf. Table 4) are about the same as the contraction numbers for the un-preconditioned W-cycle algorithm with $m = 23$ (cf. Table 5). For $k = 7$, the former takes 4.7×10^8 floating point operations and 2.1 s while the latter takes 1.1×10^9 floating point operations and 4.7 s.

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