EFFICIENT NUMERICAL METHODS FOR COMPUTING THE STATIONARY STATES OF PHASE FIELD CRYSTAL MODELS

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Abstract. Finding the stationary states of a free energy functional is an important problem in phase field crystal (PFC) models. Many efforts have been devoted for designing numerical schemes with energy dissipation and mass conservation properties. However, most existing approaches are time-consuming due to the requirement of small effective time steps. In this paper, we discretize the energy functional and propose efficient numerical algorithms for solving the constrained non-convex minimization problem. A class of first order approaches, which is the so-called adaptive accelerated Bregman proximal gradient (AA-BPG) methods, is proposed and the convergence property is established without the global Lipschitz constant requirements. Moreover, we design a hybrid approach that applies an inexact Newton method to further accelerate the local convergence. One key feature of our algorithm is that the energy dissipation and mass conservation properties hold during the iteration process. Extensive numerical experiments, including two three dimensional periodic crystals in Landau-Brazovskii (LB) model and a two dimensional quasicrystal in Lifshitz-Petrich (LP) model, demonstrate that our approaches have adaptive time steps which lead to a significant acceleration over many existing methods when computing complex structures.

Key words. Phase field crystal models, Stationary states, Quasicrystals, Projection method, Efficient iterative methods

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1. Introduction. The phase field crystal (PFC) model is an important approach to describe many physical processes and material properties, such as the formation of ordered structures, nucleation process, crystal growth, elastic and plastic deformations of the lattice, dislocations [9, 23]. More concretely, let the order parameter function be \( \phi(r) \), the PFC model can be expressed by a free energy functional

\[
E[\phi(r); \Theta] = G[\phi(r); \Theta] + F[\phi(r); \Theta],
\]

where \( \Theta \) are the physical parameters, \( F[\phi] \) is the bulk energy with polynomial type or log-type formulation and \( G[\phi] \) is the interaction energy that contains higher-order differential operators to form ordered structures [7, 18, 28]. A typical interaction potential function for a domain \( \Omega \) is

\[
G[\phi] = \frac{1}{|\Omega|} \int_{\Omega} \left( \prod_{j=1}^{m} (\Delta + q_j^2)\phi \right)^2 \, dr, \quad m \in \mathbb{N}
\]

which can be used to describe the pattern formation of periodic crystals, quasicrystals and multi-polynary crystals [18, 24, 20]. In order to understand the theory of PFC models as well as predict and guide experiments, it requires to find stationary states \( \phi_s(r; \Theta) \) and construct phase diagrams of the energy functional (1.1). Denote \( V \) to be a feasible space, the phase diagram is obtained via solving the minimization problem

\[
\min E[\phi(r); \Theta], \text{ s.t. } \phi \in V,
\]
with different physical parameters $\Theta$, which brings the tremendous computational burden. Therefore, within an appropriate spatial discretization, the goal of this paper is to develop efficient and robust numerical methods for solving (1.3) with guaranteed convergence while keeping the desired dissipation and conservation properties during the iterative process.

Most existing numerical methods for computing the stationary states of PFC models can be classified into two categories. One is to solve the steady nonlinear Euler-Lagrange equations of (1.3) through different spatial discretization approaches. The other class aims at solving the nonlinear gradient flow equation by using the numerical PDE methods. In these approaches, great efforts have been made for keeping the energy dissipation which is crucial for convergence. Typical energy stable schemes to gradient flows include convex splitting and stabilized factor methods, and recently developed invariant energy quadrature, and scalar auxiliary variable approaches for a modified energy [35, 31, 26, 36, 25]. It is noted that the gradient flow approach is able to describe the quasi-equilibrium behavior of PFC systems. Numerically, the gradient flow is discretized in both space and time domain via different discretization techniques and the stationary state is obtained with a proper choice of initialization.

Under an appropriate spatial discretization scheme, the infinite dimensional problem (1.3) can be formulated as a minimization problem in a finite dimensional space. Thus, there may exist alternative numerical methods that can converge to the steady states quickly by using modern optimization techniques. For example, similar ideas have shown success in computing steady states of the Bose-Einstein condensate [32] and the calculation of density functional theory [30, 19]. In this paper, in order to keep the mass conservation property, an additional constraint is imposed in (1.3) and the detail will be given in the next section. Inspired by the recent advances of first order methods which have been successfully applied in image processing and machine learning, we propose an adaptive accelerated Bregman proximal gradient (AA-BPG) method for computing the stationary states of (1.3). In each iteration, the AA-BPG method updates the estimation of the order parameter function by solving linear equations which have closed form when using the pseudo-spectral discretization and chooses step sizes by using the line search algorithm initialized with the Barzilai-Borwein (BB) method [2]. Meanwhile, a restart scheme is proposed such that the iterations satisfy energy dissipation property and it is proved that the generated sequence converges to a stationary point of (1.3) without the assumption of the existence of global Lipschitz constant of the bulk energy $F$. Moreover, an inexact regularized Newton method is applied for further accelerating the local convergence. More specifically, an inexact preconditioned conjugate gradient method is designed for solving the regularized Newton system efficiently. Extensive numerical experiments have demonstrated that our approach can quickly reach the vicinity of an optimal solution with moderately accuracy, even for very challenge cases.

The rest of this paper is organized as follows. In section 2, we present the PFC models considered in this paper, and the projection method discretization. In section 3, we present the AA-BPG method for solving the constrained non-convex optimization with proved convergence. In section 4, two choices of Bregman distance are proposed and applied for the PFC problems. In section 5, we design a hybrid method combining with AA-BPG methods and an inexact regularized Newton method together to further accelerate the calculation. Numerical results are reported in section 6 to illustrate the efficiency and accuracy of our algorithms. Finally, some concluding remarks are given in section 7.
2. Problem formulation.

2.1. Physical models. Two classes of PFC models are considered in the paper. The first one is the Landau-Brazovskii (LB) model which can characterize the phase and phase transitions of periodic crystals [7]. It has been discovered in many different scientific fields, e.g., polymeric materials [27]. In particular, the energy functional of LB model is

\[
E_{LB}(\phi(\mathbf{r})) = \frac{1}{|\Omega|} \int_{\Omega} \left\{ \frac{\xi^2}{2} \left[ (\Delta + 1) \phi^2 \right] + \frac{\tau}{2!} \phi^2 - \frac{\gamma}{3!} \phi^3 + \frac{1}{4!} \phi^4 \right\} \, d\mathbf{r},
\]

where \(\phi(\mathbf{r})\) is a real-valued function which measures the order of system in terms of order parameter. \(\Omega\) is the bounded domain of system, \(\xi\) is the bare correlation length, \(\tau\) is the dimensionless reduced temperature, \(\gamma\) is phenomenological coefficient. Compared with double-well bulk energy [28], the cubic term in the LB functional helps us study the first-order phase transition.

The second one is the Lifshitz-Petrich (LP) model that can simulate quasiperiodic structures, such as the bi-frequency excited Faraday wave [18], and explain the stability of soft-matter quasicrystals [17, 11]. Since quasiperiodic structures are space-filling without decay, it is necessary to define the average spacial integral over the whole space as

\[
\int = \lim_{R \to \infty} \frac{1}{|B_R|} \int_{B_R},
\]

where \(B_R \subset \mathbb{R}^d\) is the ball centred at origin with radii \(R\). The energy functional of LP model is given by

\[
E_{LP}(\phi(\mathbf{r})) = \int \left\{ \frac{c}{2} \left[ (\Delta + q_1^2)(\Delta + q_2^2) \phi^2 \right] + \frac{\varepsilon}{2} \phi^2 - \frac{\kappa}{3} \phi^3 + \frac{1}{4} \phi^4 \right\} \, d\mathbf{r},
\]

where \(c\) is the energy penalty, \(\varepsilon\) and \(\kappa\) are phenomenological coefficients.

Furthermore, we impose the following mean zero condition of order parameter on LB and LP systems to ensure the mass conservation, respectively.

\[
\frac{1}{|\Omega|} \int_{\Omega} \phi(\mathbf{r}) \, d\mathbf{r} = 0 \quad \text{or} \quad \int_{\Omega} \phi(\mathbf{r}) \, d\mathbf{r} = 0.
\]

The equality constraint condition is from the definition of the order parameter which is the deviation from average density. Besides, this equality implies that the system works in canonical ensemble such that the number of particles in the system is conserved.

2.2. Projection method discretization. In this section, we introduce the projection method [13], a high dimensional interpretation approach which can avoid the Diophantine approximation error in computing quasiperiodic systems, to discretize the LB and LP energy functional. It is noted that the stationary states in LB model is periodic, and thus it can be discretized by the Fourier pseudo-spectral method which is a special case of projection method. Therefore, we only consider the projection method discretization of the LP model (2.2). We immediately have the following orthonormal property in the average spacial integral sense

\[
\int \delta_{k, k'} \, d\mathbf{r} = \delta_{kk'}, \quad \forall \mathbf{k}, \mathbf{k}' \in \mathbb{R}^d.
\]
For a quasiperiodic function, we can define the Bohr-Fourier transformation as \[14\]
\begin{equation}
\hat{\phi}(k) = \int \phi(r)e^{-i k \cdot r} \, dr, \quad k \in \mathbb{R}^d.
\end{equation}

In this paper, we carry out the above computation in a higher dimension using the projection method which is based on the fact that a \(d\)-dimensional quasicrystal can be embedded into an \(n\)-dimensional periodic structure (\(n \geq d\)) \[10\]. The dimension \(n\) is the number of linearly independent numbers over the rational number field. Using the projection method, the order parameter \(\phi(r)\) can be expressed as
\begin{equation}
\phi(r) = \sum_{h \in \mathbb{Z}^n} \hat{\phi}(h)e^{i[(P \cdot B)h] \cdot r}, \quad r \in \mathbb{R}^d,
\end{equation}

where \(B \in \mathbb{R}^{n \times n}\) is invertible, related to the \(n\)-dimensional primitive reciprocal lattice. The corresponding computable domain in physical space is \(2\pi B^{-T} r, \tau \in [0, 1]^n\). The projection matrix \(P \in \mathbb{R}^{d \times n}\) depends on the property of quasicrystals, such as rotational symmetry \[10\]. If consider periodic crystals, the projection matrix becomes the \(d\)-order identity matrix, then the projection reduces to the common Fourier spectral method. The Fourier coefficient \(\hat{\phi}(h)\) satisfies
\begin{equation}
X := \left\{ (\hat{\phi}(h))_{h \in \mathbb{Z}^n} : \hat{\phi}(h) \in \mathbb{C}, \sum_{h \in \mathbb{Z}^n} |\hat{\phi}(h)| < \infty \right\}.
\end{equation}

In practice, let \(N = (N_1, N_2, \ldots, N_n) \in \mathbb{N}^n\), and
\begin{equation}
X_N := \{ \hat{\phi}(h) \in X : \hat{\phi}(h) = 0, \text{ for all } |h_j| > N_j/2, j = 1, 2, \ldots, n \}.
\end{equation}
The number of elements in the set is \(N = (N_1 + 1)(N_2 + 1) \cdots (N_n + 1)\). Together with \(2.4\) and \(2.6\), the discretized energy function \(2.2\) is
\begin{equation}
E_h(\hat{\Phi}) = G_h(\hat{\Phi}) + F_h(\hat{\Phi}),
\end{equation}
where \(G_h\) and \(F_h\) are the discretized interaction and bulk energies:
\begin{equation}
G_h(\hat{\Phi}) = \frac{\varepsilon}{2} \sum_{h_1 + h_2 = 0} [q_1^2 - (P \cdot B h)]^2 [q_2^2 - (P \cdot B h)]^2 \hat{\phi}(h_1) \hat{\phi}(h_2),
\end{equation}
\begin{equation}
F_h(\hat{\Phi}) = \frac{\varepsilon}{2} \sum_{h_1 + h_2 = 0} \hat{\phi}(h_1) \hat{\phi}(h_2) - \frac{\kappa}{3} \sum_{h_1 + h_2 + h_3 = 0} \hat{\phi}(h_1) \hat{\phi}(h_2) \hat{\phi}(h_3)
\end{equation}
\begin{equation}
+ \frac{1}{4} \sum_{h_1 + h_2 + h_3 + h_4 = 0} \hat{\phi}(h_1) \hat{\phi}(h_2) \hat{\phi}(h_3) \hat{\phi}(h_4),
\end{equation}
and \(h_j \in \mathbb{Z}^n\), \(\hat{\phi}_j \in X_N\), \(j = 1, 2, \ldots, 4\), \(\hat{\Phi} = (\hat{\phi}_1, \hat{\phi}_2, \ldots, \hat{\phi}_N) \in \mathbb{C}^N\). It is clear that the nonlinear terms in \(F_h\) are \(n\)-dimensional convolutions in the reciprocal space. A direct evaluation of these convolution terms is extremely expensive. Instead, these terms are simple multiplication in the \(n\)-dimensional physical space. Similar to the pseudo-spectral approach, these convolutions can be efficiently calculated through FFT. Moreover, the mass conservation constraint \(2.3\) is discretized as
\begin{equation}
\epsilon_1^T \hat{\Phi} = 0,
\end{equation}
Efficient Methods for the Stationary States of PFC Models

where \( e_1 = (1, 0, \ldots, 0) \top \in \mathbb{R}^N \). Therefore, we obtain the following finite dimensional minimization problem

\[
\min_{\hat{\Phi} \in \mathbb{C}^N} E_h(\hat{\Phi}) = G_h(\hat{\Phi}) + F_h(\hat{\Phi}), \quad \text{s.t. } e_1^\top \hat{\Phi} = 0.
\]

For simplicity, we omit the subscription in \( G_h \) and \( F_h \) in the following context. According to (2.10), denoting \( F_N \in \mathbb{C}^{N \times N} \) as the discretized Fourier transformation matrix, we have

\[
\begin{align*}
(2.13) & \quad \nabla G(\hat{\Phi}) = D\hat{\Phi}, \quad \nabla F(\hat{\Phi}) = F_N^{-1} \Lambda F_N \hat{\Phi}, \\
(2.14) & \quad \nabla^2 G(\hat{\Phi}) = D, \quad \nabla^2 F(\hat{\Phi}) = F_N^{-1} \Lambda(\cdot) F_N,
\end{align*}
\]

where \( D \) is a diagonal matrix with nonnegative entries \( c \left[ q_1^2 - (\mathcal{P}Bh)^\top (\mathcal{P}Bh) \right] \times \left[ q_2^2 - (\mathcal{P}Bh)^\top (\mathcal{P}Bh) \right] \) and \( \Lambda, \Lambda(\cdot) \in \mathbb{R}^{N \times N} \) are also diagonal matrices but related to \( \hat{\Phi} \). In the next section, we propose the adaptive accelerated Bregman proximal gradient (AA-BPG) method for solving the constrained minimization problem (2.12).

3. The AA-BPG method. Consider the minimization problem that has the form

\[
(3.1) \quad \min_x E(x) = f(x) + g(x),
\]

where \( f \in C^2 \) is proper but non-convex and \( g \) is proper, lower semi-continuous and convex. Let the domain of \( E \) to be \( \text{dom} E = \{x \mid E(x) < +\infty\} \), we make the following assumptions.

Assumption 3.1. \( E \) is bounded below and for any \( x^0 \in \text{dom} E \), the sub-level set \( \mathcal{M}(x^0) := \{x \mid E(x) \leq E(x^0)\} \) is compact.

Let \( h \) be a strongly convex function such that \( \text{dom} h \subset \text{dom} f \) and \( \text{dom} g \cap \text{intdom} h \neq \emptyset \). Then, it induces the Bregman divergence \([8]\) defined as

\[
(3.2) \quad D_h(x, y) = h(x) - h(y) - \langle \nabla h(y), x - y \rangle, \quad \forall (x, y) \in \text{dom} h \times \text{intdom} h.
\]

It is noted that \( D_h(x, y) \geq 0 \) and \( D_h(x, y) = 0 \) if and only if \( x = y \) due to the strongly convexity of \( h \). Furthermore, \( D_h(x, \bar{x}) \to 0 \) as \( x \to \bar{x} \). In recent years, Bregman distance based proximal methods \([3, 6]\) have been proposed and applied for solving the (3.1) in a general non-convex setting \([16]\). Basically, given the current estimation \( x^k \in \text{intdom} h \) and step size \( \alpha_k > 0 \), it updates \( x^{k+1} \) via

\[
(3.3) \quad x^{k+1} = \arg\min_x \left\{ g(x) + \langle x - x^k, \nabla f(x^k) \rangle + \frac{1}{\alpha_k} D_h(x, x^k) \right\}.
\]

Under suitable assumptions, it is proved in \([16]\) that the iterates \( \{x^k\} \) has similar convergence property as the traditional proximal gradient method \([4]\) while iteration (3.3) does not require the Lipschitz condition on \( \nabla f \). Motivated by the Nesterov acceleration technique \([29, 4]\), we add an extrapolation step before (3.3) and thus the iterate becomes

\[
\begin{align*}
(3.4) & \quad y^k = x^k + w_k(x^k - x^{k-1}), \\
& \quad x^{k+1} = \arg\min_x \left\{ g(x) + \langle x - y^k, \nabla f(y^k) \rangle + \frac{1}{\alpha_k} D_h(x, y^k) \right\},
\end{align*}
\]
where \( w_k \in [0, \bar{w}] \). It is noted that the minimization problems in (3.3) and (3.4) are well defined and single valued as \( g \) is convex and \( h \) is strongly convex. Although the extrapolation step accelerates the convergence in some cases, it may generate the oscillating phenomenon of the objective value \( E(x) \) that slows down the convergence [22]. Therefore, we propose a restart algorithm that leads to a convergent algorithm for solving (3.1) with energy dissipation property. Given \( \alpha_k > 0 \), define

\[
(3.5) \quad z^k = \arg\min_x \left\{ g(x) + \langle x - y^k, \nabla f(y^k) \rangle + \frac{1}{\alpha_k} D_h(x, y^k) \right\},
\]

we reset \( w_k = 0 \) if the following does not hold

\[
(3.6) \quad E(x^k) - E(z^k) \geq c\|x^k - x^{k+1}\|^2
\]

for some constant \( c > 0 \). In the next section, we will show that (3.6) holds when \( w_k = 0 \). Overall, the AA-BPG algorithm is presented in Algorithm 3.1.

**Step size estimation.** In each step, \( \alpha_k \) is chosen adaptively by backtracking linear search method which is initialized by the BB step [2] estimation, i.e.

\[
(3.7) \quad \alpha_k = \frac{s_k}{s_k^T v_k} \text{ or } \frac{v_k}{s_k^T v_k},
\]

where \( s_k = x^k - x^{k-1} \) and \( v_k = \nabla f(x^k) - \nabla f(x^{k-1}) \). Let \( \eta > 0 \) be a small constant and \( z^k \) be obtained from (3.5), we adopt the step size \( \alpha_k \) whenever the following inequality holds

\[
(3.8) \quad E(y^k) - E(z^k) \geq \eta\|y^k - z^k\|^2.
\]

The detailed estimation method is presented in Algorithm 3.2.

### Algorithm 3.1 AA-BPG Algorithm

**Require:** \( x^1 = x^0, \alpha_0 > 0, w_0 \in [0, 1], \rho \in (0, 1), \eta, c > 0 \) and \( \bar{w} > 0 \)

1. while the stop criterion is not satisfied do
2. \quad Update \( w_k \in [0, \bar{w}] \)
3. \quad Update \( y^k = x^k + w_k(x^k - x^{k-1}) \)
4. \quad Estimate \( \alpha_k \) by Algorithm 3.2
5. \quad Calculate \( z^k \) via (3.5)
6. \quad if (3.6) holds then
7. \quad \quad \( x^{k+1} = z^k \).
8. \quad else
9. \quad \quad Reset \( w_k = 0 \).
10. \quad end if
11. \quad \( k = k + 1 \).
12. end while

### 3.1. Convergence analysis.** In this section, we focus on the convergence analysis of the proposed AA-BGP method. Before proceeding, we introduce some definitions used in analysis.
3.2. Definitions.

**Definition 3.1.** Let $g$ be a proper and lower semi-continuous function and convex function. The subgradient of $g$ at $x \in \text{dom} g$ is defined as

$$\partial g(x) = \{ u : f(y) - f(x) - \langle u, y - x \rangle \geq 0, \forall y \in \text{dom} g \}.$$ 

**Definition 3.2.** $x$ is called a stationary point of $E$ if

$$0 \in \partial E(x) = \nabla f(x) + \partial g(x).$$

**Definition 3.3.** A function $f \in C^2$ is $L_f$-relative smooth if there exists a strongly convex function $h \in C^2$ such that

$$L_f \nabla^2 h(x) - \nabla^2 f(x) \succeq 0, \quad \forall x \in \text{intdom} h. \quad (3.9)$$

**Algorithm 3.2** Estimation of $\alpha_k$ at $y^k$

**Require:** $x^k, y^k, \eta > 0$ and $\rho \in (0, 1)$ and $\alpha_{\min}, \alpha_{\max} > 0$

1. Initialize $\alpha_k$ by BB step (3.7).
2. for $j = 1, 2, \ldots$ do
3. Calculate $z^k$ via (3.5)
4. if (3.8) holds or $\alpha_k < \alpha_{\min}$ then
5. break
6. else
7. $\alpha_k = \rho \alpha_k$
8. end if
9. end for
10. Output $\alpha_k = \max(\min(\alpha_k, \alpha_{\max}), \alpha_{\min})$.

3.3. Convergence property. Throughout this section, we impose the next assumption on $f$.

**Assumption 3.2.** There exists $L_f > 0$ such that $f$ is $L_f$-relative smooth with respect to a strongly convex function $h \in C^2$.

Under the Assumption 3.2, we have the following useful lemma as stated in [3].

**Lemma 3.4 ([3]).** If $f$ is $L_f$-relative smooth with respect to $h$, then

$$f(x) - f(y) - \langle \nabla f(y), x - y \rangle \leq L_f D_h(x, y), \quad \forall x, y \in \text{intdom} h. \quad (3.10)$$

Based on the above Lemma, the descent property of the iteration generated by Bregman proximal operator (3.5) is established as follows.

**Lemma 3.5.** Let $\alpha > 0$ and suppose the Assumption 3.2 holds. If

$$z = \arg\min_x \left\{ g(x) + \langle x - y, \nabla f(y) \rangle + \frac{1}{\alpha} D_h(x, y) \right\}, \quad (3.11)$$

then there exists some $\sigma > 0$ such that

$$E(y) - E(z) \geq \left( \frac{1}{\alpha} - L_f \right) \frac{\sigma}{2} \| z - y \|^2. \quad (3.12)$$
Proof. Since \( h \) is strongly convex, there exists some constant \( \sigma > 0 \) such that \( h(x) - \sigma \|x\|^2/2 \) is convex. Then, \( \nabla^2 h(x) - \sigma I \succeq 0 \) and we have

\[
D_h(z, x) = h(z) - h(y) - \langle \nabla h(y), z - y \rangle \geq \frac{\sigma}{2} \|z - y\|^2.
\]

From the optimal condition of (3.11), we have

\[
E(y) = f(y) + g(y) = \left[ f(y) + \langle \nabla f(y), x - y \rangle + \frac{1}{\alpha} D_h(x, y) + g(x) \right]_{x=y}
\geq f(y) + \langle \nabla f(y), z - y \rangle + \frac{1}{\alpha} D_h(z, y) + g(z)
\geq f(z) - L_f D_h(z, y) + \frac{1}{\alpha} D_h(z, y) + g(z)
= E(z) + \left( \frac{1}{\alpha} - L_f \right) D_h(z, y) \geq E(z) + \left( \frac{1}{\alpha} - L_f \right) \frac{\sigma}{2} \|z - y\|^2,
\]

where the second inequality is from (3.10) and the last inequality follows from (3.13).[]

Remark 3.3. Lemma 3.5 shows that the non-restart condition (3.6) and the linear search condition (3.8) are satisfied when

\[
0 < \alpha < \bar{\alpha} := \min \left( \frac{1}{2e/\sigma + L_f}, \frac{1}{2\eta/\sigma + L_f} \right) \quad \text{and} \quad 0 < \alpha_{\text{min}} \leq \bar{\alpha}
\]

Therefore, the line search in Algorithm 3.2 stops in finite iterations, and thus the Algorithm 3.1 is well defined.

In the following analysis, we always assume that the parameter \( \alpha_{\text{min}} \) satisfies (3.14) for simplicity. Therefore, we can obtain the sufficient decrease property of the sequence generated by Algorithm 3.1.

Corollary 3.6. Suppose the Assumption 3.1 and Assumption 3.2 hold. Let \( \{x^k\} \) be the sequence generated by the Algorithm 3.1. Then, \( \{x^k\} \subset M(x^0) \) and

\[
E(x^k) - E(x^{k+1}) \geq c_0 \|x^k - x^{k+1}\|^2,
\]

where \( c_0 = \min(c, \eta) \).

The proof of Corollary 3.6 is a straightforward result as AA-BPG algorithm is well defined and the condition (3.6) or (3.8) holds at each iteration. Let \( B(x^0) \) be the closed ball that contains \( M(x^0) \). Since \( h, F \in C^2 \), there exist \( \rho_h, \rho_f > 0 \) such that

\[
\rho_h = \sup_{x \in B(x^0)} \|\nabla^2 h(x)\|, \quad \rho_f = \sup_{x \in B(x^0)} \|\nabla^2 f(x)\|.
\]

Thus, we can show the subgradient of each step generated by Algorithm 3.1 is bounded by the movement of \( x^k \).

Lemma 3.7 (Bounded the subgradient). Suppose Assumption 3.1 and Assumption 3.2 holds. Let \( \{x^k\} \) be the sequence generated by Algorithm 3.1. Then, there exists \( c_1 = \rho_f + \rho_h/\alpha_{\text{min}} > 0 \) such that

\[
\text{dist}(0, \partial E(x^{k+1})) \leq c_1 (\|x^{k+1} - x^k\| + \bar{w} \|x^k - x^{k-1}\|),
\]

where \( \text{dist}(0, \partial E(x^{k+1})) = \inf \{\|y\| : y \in \partial E(x^{k+1})\} \) and \( \rho_h, \rho_f \) are defined as (3.16) and \( \bar{w}, \alpha_{\text{min}} \) are constants defined in Algorithm 3.1 and Algorithm 3.2, respectively.
Proof. By the first order optimality condition of (3.4), we get
\[
0 \in \nabla f(y^k) + \frac{1}{\alpha_k} (\nabla h(x^{k+1}) - \nabla h(y^k)) + \partial g(x^{k+1})
\]
\[
\iff - \nabla f(y^k) - \frac{1}{\alpha_k} (\nabla h(x^{k+1}) - \nabla h(y^k)) \in \partial g(x^{k+1})
\]
From Lemma 3.5, we have \(x^k, x^{k-1} \in \mathcal{M}(0^0)\), then \(y^k = (1+w_k)x^k - w_kx^{k-1} \in \mathcal{B}(0^0)\).
It follows that
\[
\text{dist}(0, \partial E(x^{k+1})) = \inf_{y \in \partial g(x^{k+1})} \| \nabla f(x^{k+1}) + y \|
\leq \| \nabla f(x^{k+1}) - \nabla f(y^k) - \frac{1}{\alpha_k} (\nabla h(x^{k+1}) - \nabla h(y^k)) \|
\leq \| \nabla f(x^{k+1}) - \nabla f(y^k) \| + \frac{1}{\alpha_k} \| \nabla h(x^{k+1}) - \nabla h(y^k) \|
\leq (\rho_f + \frac{\rho_h}{\alpha_k})\|x^{k+1} - y^k\|
\leq c_1(\|x^{k+1} - x^k\| + \bar{w}\|x^k - x^{k-1}\|),
\]
where the last inequality is from \(y^k = x^k + w_k(x^k - x^{k-1})\) and \(w_k \in [0, \bar{w}]\).

Now, we are ready to establish the sub-convergence property of Algorithm 3.1.

**Theorem 3.4.** Suppose Assumption 3.1 and Assumption 3.2 hold. Let \(\{x^k\}\) be the sequence generated by Algorithm 3.1. Then, for any limit point \(x^*\) of \(\{x^k\}\), we have \(0 \in \partial E(x^*)\).

**Proof.** From Corollary 3.6, we know \(\{x^k\} \subset \mathcal{M}(0^0) \subset \mathcal{B}(0^0)\) and thus bounded. Then, the set of limit points of \(\{x^k\}\) is nonempty. For any limit point \(x^*\), there exist a subsequence \(\{x^{k_j}\}\) such that \(x^{k_j} \to x^*\) as \(j \to \infty\). We know \(\{E(x^j)\}\) is a decreasing sequence. Together with the fact that \(E\) is bounded below, there exists some \(\bar{E}\) such that \(E(x^k) \to \bar{E}\) as \(k \to \infty\). Moreover, it has
\[
E(0^0) - \bar{E} = \lim_{K \to \infty} \sum_{j=0}^{K} (E(x^j) - E(x^{j+1})) \geq c_0 \lim_{K \to \infty} \sum_{j=0}^{K} \|x^j - x^{j+1}\|^2,
\]
and implies \(\|x^k - x^{k-1}\| \to 0\) as \(k \to \infty\). As a result,
\[
\lim_{k \to \infty} \|x^k - y^{k-1}\| \leq \lim_{k \to \infty} (\|x^k - x^{k-1}\| + \bar{w}\|x^{k-1} - x^{k-2}\|) = 0.
\]
Together with (3.17), it implies that there exists \(u^{k_j} \in \partial g(x^{k_j})\) such that
\[
\lim_{j \to \infty} \|\nabla f(x^{k_j}) + u^{k_j}\| = 0 \Rightarrow \lim_{j \to \infty} u^{k_j} = -\nabla f(x^*),
\]
as \(\nabla f\) is continuous and \(x^{k_j} \to x^*\) when \(j \to \infty\).

In the next, we prove \(\lim_{j \to \infty} g(x^{k_j}) = g(x^*)\). It is easy to know that \(\lim_{j \to \infty} x^{k_j-p} = x^*\) for finite \(p \geq 0\) since \(\lim_{k \to \infty} \|x^k - x^{k-1}\| = 0\). Thus, we have \(y^{k_j-1} = x^{k_j-1} + u_{k_j-1}(x^{k_j-1} - x^{k_j-2}) \to x^*\) as \(j \to \infty\). From (3.4), we know
\[
g(x^{k_j}) + \langle x^{k_j} - y^{k_j-1}, \nabla f(y^{k_j-1}) \rangle + \frac{1}{\alpha_k} D(x^{k_j}, y^{k_j-1})
\leq g(x) + \langle x - y^{k_j-1}, \nabla f(y^{k_j-1}) \rangle + \frac{1}{\alpha_k} D(x, y^{k_j-1}), \ \forall x.
\]
Let \( x = x^* \) and \( j \to \infty \), we get \( \limsup_{j \to \infty} g(x^{kj}) \leq g(x^*) \). By the fact that \( g(x) \) is lower semi-continuous, it has \( \lim_{j \to \infty} g(x^{kj}) = g(x^*) \).

Thus, by the convexity of \( g \), we have

\[
g(x) \geq g(x^{kj}) + \langle u^{kj}, x - x^{kj} \rangle, \forall x \in \text{dom}\, g.
\]

Let \( j \to \infty \) in (3.21) and using the facts \( x^{kj} \to x^* \), \( g(x^{kj}) \to g(x^*) \) as \( j \to \infty \) and (3.19), we have \(-\nabla f(x^*) \in \partial g(x^*)\) and thus \( 0 \in \partial g(x^*) \).

Furthermore, the sub-sequence convergence can be strengthen by imposing the next assumption on \( E \) which is known as the Kurdyka-Lojasiewicz (KL) property [5].

**Assumption 3.5.** \( E(x) \) is the KL function, i.e. for all \( \bar{x} \in \text{dom}\, E := \{x : \partial E(x) \neq \emptyset\} \), there exist \( \eta > 0 \), a neighborhood \( U \) of \( \bar{u} \) and \( \psi \in \Psi_\eta := \{\psi \in C[0, \eta] \cap C_1(0, \eta), \psi \text{ is concave, } \psi(0) = 0, \psi' > 0 \text{ on } (0, \eta)\} \) such that for all \( x \in U \cap \{x : E(x) < E(\bar{x}) \leq E(\bar{x}) + \eta\} \), the following inequality holds,

\[
\psi'(E(x) - E(\bar{x})) \operatorname{dist}(0, \partial E(x)) \geq 1.
\]

**Theorem 3.6.** Suppose Assumption 3.1, Assumption 3.2 and Assumption 3.5 hold. Let \( \{x^k\} \) be the sequence generated by Algorithm 3.1. Then, there exists a point \( x^* \in \mathcal{B}(x^0) \) such that

\[
\lim_{k \to +\infty} x^k = x^*, \quad 0 \in \partial E(x^*).
\]

**Proof.** The proof is in Appendix A.

It is known from [5] that many functions satisfy Assumption 3.5 including the energy function in PFC models. In the following context, we apply the AA-BPG method for solving the PFC models (2.12) by introducing two Bregman distances.

### 4. AA-BPG method for solving PFC models

The problem (2.12) can be reduced to (3.1) by setting

\[
f(\hat{\Phi}) = F(\hat{\Phi}), \quad g(\hat{\Phi}) = G(\hat{\Phi}) + \delta_S(\hat{\Phi})
\]

where \( S = \{\hat{\Phi} : e_i^\top \hat{\Phi} = 0\} \) and \( \delta_S(\hat{\Phi}) = 0 \) if \( \hat{\Phi} \in S \) and \(+\infty\) otherwise. The main difficulty of applying Algorithm 3.1 is solving the subproblem (3.5) efficiently. In this section, two different strongly convex functions \( h \) are chosen as

\[
h(x) = \frac{1}{2} \|x\|^2 \quad \text{(P2)} \quad \text{and} \quad h(x) = \frac{a}{4} \|x\|^4 + \frac{b}{2} \|x\|^2 + 1 \quad \text{(P4)},
\]

where \( a, b > 0 \) and (P2) and (P4) represent the highest order of the \( l^2 \) norm.

**Case (P2).** The Bregman distance of \( D_h \) is reduced to the Euclidean distance, i.e.

\[
D_h(x, y) = \frac{1}{2} \|x - y\|^2.
\]

The subproblem (3.5) is reduced to

\[
\min_{\hat{\Phi}} G(\hat{\Phi}) + \langle \nabla F(\hat{\Phi}), \hat{\Phi} - \hat{\Psi} \rangle + \frac{1}{2\alpha} \|\hat{\Phi} - \hat{\Psi} \|^2, \text{ s.t. } e_i^\top \hat{\Phi} = 0,
\]

where \( \hat{\Psi} = \hat{\Phi} + w_k(\hat{\Phi} - \hat{\Psi}^{k-1}) \). Although the (4.4) is a constrained minimization problem, it has a closed form solution based on our discretization which leads to a fast computation.
Lemma 4.1. Given $\alpha_k > 0$, if $e_1^T \hat{\Psi} = 0$, the minimizer of (4.4), denoted by $\hat{\Phi}^{k+1}$, is given by

$$
(4.5) \quad \hat{\Phi}^{k+1} = (I + \alpha_k D)^{-1} \left( \hat{\Psi}^k - \alpha_k P_1 \nabla F(\hat{\Psi}^k) \right),
$$

where $D$ is defined in (2.13) and $P_1 = I - e_1 e_1^T$ is the projection into the set $S$.

Proof. The KKT conditions for this subproblem (3.5) can be written as

$$
(4.6) \quad \nabla G(\hat{\Phi}^{k+1}) + \nabla F(\hat{\Psi}^k) + \frac{1}{\alpha_k} \left( \hat{\Phi}^{k+1} - \hat{\Psi}^k \right) - \xi_k e_1 = 0,
$$

(4.7) $e_1^T \hat{\Phi}^{k+1} = 0,$

where $\xi_k$ is the Lagrange multiplier. Taking the inner product with $e_1$ in (4.6), we obtain

$$
\xi_k = e_1^T \left( \nabla G(\hat{\Phi}^{k+1}) + \nabla F(\hat{\Psi}^k) - \frac{1}{\alpha_k} \hat{\Psi}^k \right).
$$

Using (4.7) and (2.13), we know

$$
e_1^T \nabla G(\hat{\Phi}^{k+1}) = e_1^T (D \hat{\Phi}^{k+1}) = 0.
$$

Together with $e_1^T \hat{\Psi}^k = 0$, we have $\xi_k = e_1^T \nabla F(\hat{\Psi}^k)$. Substituting it into (4.6), it follows that

$$
\hat{\Phi}^{k+1} = (\alpha_k D + I)^{-1} \left( \hat{\Psi}^k - \alpha_k P_1 \nabla F(\hat{\Psi}^k) \right).
$$

It is noted that from the proof of Lemma 4.1, the feasibility assumption $e_1^T \hat{\Psi} = 0$ holds as long as $e_1^T \hat{\Phi} = 0$ which can be set in the initialization. The detailed algorithm is given in Algorithm 4.1 with $K = 2$.

Case (P4). In this case, the subproblem (3.5) is reduced to

$$
(4.8) \quad \min_\Phi G(\hat{\Phi}) + (\nabla F(\hat{\Psi}^k), \Phi - \hat{\Psi}^k) + D_h(\Phi, \hat{\Psi}^k), \text{ s.t. } e_1^T \Phi = 0.
$$

where $\hat{\Psi}^k = \hat{\Phi}^k + w_h(\hat{\Phi}^k - \hat{\Psi}^{k-1})$. The next lemma shows the optimal condition of minimizing (4.8).

Lemma 4.2. Given $\alpha_k > 0$. If $e_1^T \hat{\Psi}^k = 0$, the minimizer of (4.8), denoted by $\hat{\Phi}^{k+1}$, is given by

$$
(4.9) \quad \hat{\Phi}^{k+1} = [\alpha_k D + (a p^* + b) I]^{-1} (\nabla h(\hat{\Psi}^k) - \alpha_k P_1 \nabla F(\hat{\Psi}^k)),
$$

where $D$ is given in (2.13) and $p^*$ is a fixed point of $p = \|\hat{\Phi}^{k+1}\|^2 := r(p)$.

Proof. The KKT conditions of (4.8) imply that there exists a Lagrange multiplier $\xi_k$ such that $(\hat{\Phi}^{k+1}, \xi_k)$ satisfies

$$
(4.10) \quad \alpha_k \nabla G(\hat{\Phi}^{k+1}) + \alpha_k \nabla F(\hat{\Psi}^k) + \nabla h(\hat{\Phi}^{k+1}) - \nabla h(\hat{\Psi}^k) - \xi_k e_1 = 0,
$$

(4.11) $e_1^T \hat{\Phi}^{k+1} = 0.$

Since $e_1^T \hat{\Phi} = 0$ and $\nabla h(x) = (a \|x\|^2 + b) x$, (4.11) and (2.13) imply

$$
e_1^T \nabla G(\hat{\Psi}^{k+1}) = e_1^T (D \hat{\Phi}^{k+1}) = 0, \quad e_1^T \nabla h(\hat{\Psi}^k) = (a \|\hat{\Psi}^k\|^2 + b) e_1^T \hat{\Psi}^k = 0,$$
where $D$ is defined in (2.13). Substituting the above equalities into (4.10) implies $\xi_k = \alpha_k e_1^T \nabla F(\hat{\Psi}^k)$. Denote

$$p := \|\hat{\Phi}^{k+1}\|^2 \geq 0, \quad \beta := \nabla h(\hat{\Psi}^k) - \alpha_k \nabla F(\hat{\Psi}^k) + \xi e_1 = \nabla h(\hat{\Psi}^k) - \alpha_k P_1 \nabla F(\hat{\Psi}^k).$$

From (4.10), we obtain a fixed point problem with respect to $p$

$$p = \|\hat{\Phi}^{k+1}\|^2 = \|D + (ap + b)I\|^{-1} \beta := r(p).$$

Let $R(p) = r(p) - p$. Then $R(0) = \|(D + bI)^{-1} \beta\|^2 \geq 0$, $R(p) \to -\infty$ as $p \to \infty$ and

$$R'(p) = -2a \sum_{i=1}^{n} \frac{\beta_i^2}{(D_i + ap + b)^3} - 1 < 0, \quad \forall p \geq 0,$$

there is an unique zero $p^* \geq 0$ of $R(p)$, i.e. $p^* = r(p^*)$. Thus,

$$\hat{\Phi}^{k+1} = [\alpha_k D + (ap^* + b)I]^{-1}(\nabla h(\hat{\Psi}^k) - \alpha_k P_1 \nabla F(\hat{\Psi}^k)).$$

It is noted that the fixed point equation (4.12) is a nonlinear scalar equation which can efficiently solved by many existing solvers. The detailed algorithm is given in Algorithm 4.1 with $K = 4$.

### Algorithm 4.1 AA-BPG-K method for PFC model

**Require:** $\hat{\Phi}^0 = \hat{\Phi}^0$, $\alpha_0 > 0$, $w_0 \in [0, 1]$, $\rho \in (0, 1)$, $\eta > c > 0$ and $\bar{w} > 0$

1. **while** stop criterion is not satisfied **do**
   2. Update $w_k \in [0, \bar{w}]$
   3. Update $\hat{\Psi}^k = \hat{\Phi}^k - w_k(\hat{\Phi}^k - \hat{\Phi}^{k-1})$
   4. Estimate $\alpha_k$ by Algorithm 3.2
   5. **if** $K = 2$ **then**
   6. Calculate $z^k = (\alpha_k D + I)^{-1} \left(\hat{\Phi}^k - \alpha_k P_1 \nabla F(\hat{\Psi}^k)\right)$
   7. **else if** $K = 4$ **then**
   8. Calculate the fixed point of (4.12).
   9. Calculate $z^k = (\alpha_k D + (a \bar{p}^* + b)I)^{-1}(\nabla h(\hat{\Psi}^k) - \alpha_k P_1 \nabla F(\hat{\Psi}^k))$
   10. **end if**
   11. **if** $E(\hat{\Psi}^k) - E(z^k) \geq c \|\hat{\Phi}^k - z^k\|^2$ **then**
   12. $\hat{\Phi}^{k+1} = z^k$.
   13. **else**
   14. Reset $w_k = 0$.
   15. **end if**
   16. $k = k + 1$.
   17. **end while**

#### 4.1. Convergence analysis for Algorithm 4.1.

The convergence analysis can be directly applied for Algorithm 4.1 if the assumptions required in Theorem 3.4 hold. We first show that the energy function $E$ in PFC model satisfies Assumption 3.1 and Assumption 3.5. Then, Assumption 3.2 is analyzed for Case (P2) and Case (P4) independently.

**Lemma 4.3.** Let $E_0 = F(\hat{\Phi}) + G(\hat{\Phi})$ and $E(\hat{\Phi}) = E_0(\hat{\Phi}) + \delta_S(\hat{\Phi})$ be the energy functional which is defined in (4.1). Then, it satisfies

1. $E$ is bounded below and the sub-level set $M(\hat{\Phi}^0)$ is compact for any $\hat{\Phi}^0 \in S$. 


2. \( E \) is a KL function, and thus satisfies Assumption 3.5.

Proof. From the continuity and the coercive property of \( F \), i.e. \( F(\check{\Phi}) \rightarrow +\infty \) as \( \check{\Phi} \rightarrow \infty \), the sub-level set \( \mathcal{S}_0 := \{ \check{\Phi} : E_0(\check{\Phi}) \leq E_0(\check{\Phi}^0) \} \) is compact for any \( \check{\Phi}^0 \). Together with \( \mathcal{S} \) is closed, it follows that \( \mathcal{M}(\check{\Phi}^0) = \mathcal{S} \cap \mathcal{S}_0 \) is compact for any \( \check{\Phi}^0 \).

Moreover, according to Example 2 in [5], it is easy to know that \( E(\check{\Phi}) \) is semi-algebraic function, then it is KL function by Theorem 2 in [5].

Lemma 4.4. Let \( F(\check{\Phi}) \) be defined in (2.12). Then, we have

1. If \( h \) is chosen as (P2) in (4.2), then \( F \) is relative smooth with respect to \( h \) in \( \mathcal{M} \) for any compact set \( \mathcal{M} \).
2. If \( h \) is chosen as (P4) in (4.2), then \( F \) is relative smooth with respect to \( h \).

Proof. Denote \( \check{\Phi}^{\otimes k} := \check{\Phi} \otimes \check{\Phi} \otimes \cdots \otimes \check{\Phi} \) where \( \otimes \) is the tensor product. Then, \( F(\check{\Phi}) \) is the 4th-degree polynomial, i.e. \( F(\check{\Phi}) = \sum_{k=2}^{4} \langle A_k, \check{\Phi}^{\otimes k} \rangle \) where the \( k \)th-degree monomials are arranged as a \( k \)th-order tensor \( A_k \). For any compact set \( \mathcal{M} \), \( \nabla^2 F \) is bounded and thus \( F \) is relative smooth with respect to any polynomial function in \( \mathcal{M} \) which includes case (P2). When \( h \) is chosen as (P4), according to Lemma 2.1 in [16], there exists \( L_F > 0 \) such that \( F(\check{\Phi}) \) is \( L_F \)-relative smooth with respect to \( h(x) \).

Combining Lemma 4.3, Lemma 4.4 with Theorem 3.6, we can directly establish the convergence of Algorithm 4.1.

Theorem 4.1. Let \( E(\check{\Phi}) = F(\check{\Phi}) + G(\check{\Phi}) + \delta_S(\check{\Phi}) \) be the energy function which is defined in (4.1). The following results hold.

1. Let \( \{ \hat{\Phi}^k \} \) be the sequence generated by Algorithm 4.1 with \( K = 2 \). If \( \{ \hat{\Phi}^k \} \) is bounded, then \( \{ \hat{\Phi}^k \} \) converges to some \( \hat{\Phi}^* \) and \( 0 \in \partial E(\hat{\Phi}^*) \).
2. Let \( \{ \hat{\Phi}^k \} \) be the sequence generated by Algorithm 4.1 with \( K = 4 \). Then, \( \{ \hat{\Phi}^k \} \) converges to some \( \hat{\Phi}^* \) and \( 0 \in \partial E(\hat{\Phi}^*) \).

It is noted that when \( h \) is chosen as (P2), we cannot bounded the growth of \( F \) as \( F \) is a fourth order polynomial. Thus, the boundedness assumption of \( \{ \hat{\Phi}^k \} \) is imposed which is similar to the requirement in the semi-implicit scheme [26].

5. Hybrid method. Despite the fast initial convergence speed of the first order methods, the tail convergence speed can be slow. Therefore it can be further locally accelerated by the feature of Newton-type methods. In this section, we first introduce an inexact Newton method that solves the PFC models (2.12) and then provide a hybrid method that automatically switches between AA-BPG and inexact Newton-PCG method.

5.1. Inexact Newton-PCG method. Define \( Z := [0, I_{N-1}]^\top \), any vector \( \check{\Phi} \) that satisfies the constraint \( e_1\check{\Phi} = 0 \) has the form of \( \check{\Phi} = ZU \) with \( U \in \mathbb{C}^{N-1} \). Since \( Z^\top Z = I_{N-1} \), we can also obtain \( U \) from \( \check{\Phi} \) by \( U = Z^\top \check{\Phi} \). Therefore, the problem (2.12) is equivalent to

\[
\min_{U \in \mathbb{C}^{N-1}} E(ZU) = G(ZU) + F(ZU).
\]

Let \( \tilde{E}(U) := E(ZU) \), \( \tilde{G}(U) := E(ZU) \), \( \tilde{F}(U) := F(ZU) \), we have the following facts

\[
\begin{align*}
\tilde{g} &:= \nabla \tilde{E}(U) = Z^\top \nabla E(ZU) = Z^\top g, \\
\tilde{J} &:= \nabla^2 \tilde{E}(U) = Z^\top \nabla^2 E(ZU)Z = Z^\top J Z,
\end{align*}
\]

where \( g = \nabla E(ZU) \) and \( J = \nabla^2 E(ZU) \). Therefore, finding the steady states of PFC models is equivalent to solving the nonlinear equations

\[
\nabla \tilde{E}(U) = 0.
\]
Due to the non-convexity of $\hat{E}(U)$, the Hessian matrix $\hat{J}$ may not be positive definite and thus a regularized Newton method is applied.

**Computing Inexact Newton direction.** Denote $\hat{J}_k := \nabla^2 \hat{E}(U^k)$ and $\hat{g}_k := \nabla \hat{E}(U^k)$. We find the approximated Newton direction $d_k$ by solving

\begin{equation}
(\hat{J}_k + \mu_k I)d_k = -\hat{g}_k,
\end{equation}

where regularized parameter $\mu_k$ is chosen as

\begin{equation}
- c_1 \min\{0, \lambda_{\min}(\hat{J}_k)\} + c_2 \|\hat{g}_k\| \leq \mu_k \leq \bar{\mu} < +\infty \quad (c_1 \geq 1, c_2 > 0).
\end{equation}

Thus, (5.4) is symmetric, positive definite linear system. To accelerate the convergence, an inexact preconditioned conjugate gradient (PCG) method is adopted. More specifically, in $k$-th step, we terminate the PCG iterates whenever $\| (\hat{J}_k + \mu_k I)d_k + \hat{g}_k \| \leq \eta_k$ in which $\eta_k$ is set as

\begin{equation}
\eta_k = \tau \min\{1, \|\hat{g}_k\|\}, \quad 0 < \tau < 1,
\end{equation}

and the preconditioner $M_k$ is adaptively obtained by setting

\begin{equation}
M_k = Z(H_k + \mu_k I)^{-1}Z^T \quad \text{with} \quad H_k = D + \delta_k I
\end{equation}

where $D$ is from (2.13) and some $\delta_k > 0$. Let $A = \hat{J}_k + \mu_k I$, $b = -\hat{g}_k$ and $M = M_k$, the inexact PCG method is given in Algorithm 5.1, where $\|x\|_A := \langle x, Ax \rangle$.

**Algorithm 5.1 PCG($\eta$) for solving $Ax = b$.**

**Require:** $A, b, \eta, k_{\text{max}}, \text{preconditioner } M$.

1. Set $x^0 = 0, r^0 = Ax^0 - b = -b, p_0 = -M^{-1}r^0, i = 0$.
2. **while** $\|r_i\| > \eta$ or $i < k_{\text{max}}$ **do**
   3. $\alpha_{i+1} = \frac{\|r_i\|^2 M^{-1}}{\|p_i\|^2 A}$
   4. $x^{i+1} = x^i + \alpha_{i+1}p_i$
   5. $r_{i+1} = r_i + \alpha_{i+1}Ap_i$
   6. $\beta_{i+1} = \frac{\|r_{i+1}\|^2 M^{-1}}{\|r_i\|^2 M^{-1}}$
   7. $p_{i+1} = -M^{-1}r_{i+1} + \beta_{i+1}p_i$
   8. $i = i + 1$
3. **end while**

**Computing the step size** $t_k$: Once the Newton direction $d_k$ is obtained, the line search technique is applied for finding an appropriate step size $t_k$ that satisfies the following inequality:

\begin{equation}
\hat{E}(U^k + t_k d_k) \leq \hat{E}(U^k) + \nu t_k \langle \hat{g}_k, d_k \rangle, \quad 0 < \nu < 1.
\end{equation}

The existence of $t_k > 0$ that satisfies (5.8) is given in Lemma 5.3. Then, $U^{k+1}$ is updated by $U^{k+1} = U^k + t_k d_k$. Our proposed algorithm is summarized in Algorithm 5.2.
5.2. Convergence analysis for Algorithm 5.2. We first establish several properties related to the direction $d_k$ computed by the inexact PCG method.

**Lemma 5.1.** Consider a linear system $Ax = b$ where $A$ is symmetric and positive definite. Let $\{x^i\}$ be the sequence generated by Algorithm 5.1, it satisfies

\[
\frac{1}{\lambda_{\text{max}}(A)} \leq \frac{\langle x^i, b \rangle}{\|b\|^2} \leq \frac{1}{\lambda_{\text{min}}(A)}, \quad \forall i = 1, 2, \ldots.
\]  

**Proof.** The proof is in Appendix B.

Then, we know the $d_k$ is a descent direction from the next lemma.

**Lemma 5.2 (Descent direction).** Let $d_k$ be generated by PCG($\eta_k$) method (Algorithm 5.1). If $\|\tilde{g}_k\| > 0$, then we have

\[
-(d_k, \tilde{g}_k) \geq l_k := \frac{\|\tilde{g}_k\|^2}{\lambda_{\text{max}}(\tilde{\mathcal{J}}_k + \mu_k I)} \quad \text{and} \quad \|d_k\| \leq \bar{d} := \frac{\tau + 1}{c_2},
\]

where $\tau$, $K$, and $c_1, c_2$ are defined in (5.6), (5.15) and (5.5), respectively.

**Proof.** The first inequality is a direct consequence of Lemma 5.1. Moreover, let $r_k = (\tilde{\mathcal{J}}_k + \mu_k I)d_k + \tilde{g}_k$. By Algorithm 5.1 and (5.6), we have $\|r_k\| \leq \eta_k \leq \tau \|\tilde{g}_k\|$. Then,

\[
\|d_k\| = \|(\tilde{\mathcal{J}}_k + \mu_k I)^{-1}(r_k - \tilde{g}_k)\| \leq \frac{\|r_k - \tilde{g}_k\|}{\lambda_{\text{min}}(\tilde{\mathcal{J}}_k + \mu_k I)} \leq \frac{\|r_k\| + \|\tilde{g}_k\|}{c_2\|g_k\|} \leq \frac{\tau + 1}{c_2},
\]

where the second inequality is from (5.5).

**Lemma 5.3 (Lower bound of $t_k$).** Let $d_k$ be generated by PCG($\eta_k$) method (Algorithm 5.1). If $\|\tilde{g}_k\| \geq \varepsilon > 0$, then for any $\nu \in (0, 1)$, there exists $M_k > 0$ and

\[
(t_k^\text{max}) := \min \left\{ \frac{2(1-\nu)\delta_k}{M_k d^2}, 1 \right\},
\]

such that the inequality (5.8) holds for $t_k \in (0, t_k^\text{max}]$ where $l_k$ is defined in (5.10).
Proof. By the Taylor expansion, we have
\[ \tilde{E}(U^k + td_k) = \tilde{E}(U^k) + t \langle \tilde{g}_k, d_k \rangle + \frac{t^2}{2} \langle d_k, \nabla^2 \tilde{E}(\xi_t) d_k \rangle, \]
where \( \xi_t \in V_k = \{V|V = U^k + td_k, t \in [0, 1]\} \). As \( \tilde{E} \in C^2 \), there exists \( M_k > 0 \) such that \( M_k = \sup \{\|\nabla^2 \tilde{E}(V)\|; \forall V \in V_k\} \). Then, (5.12) and (5.10) imply
\[ \tilde{E}(U^k + td_k) \leq \tilde{E}(U^k) + \nu t \langle \tilde{g}_k, d_k \rangle - (1 - \nu)l_k t + \frac{M_k d^2 t^2}{2}. \]
Define \( Q(t) = (1 - \nu)l_k t - \frac{M_k d^2 t^2}{2}, \) we know \( Q(t) \geq 0 \) for all \( t \in [0, \frac{2(1 - \nu)l_k}{M_k d^2}] \) which implies (5.8) holds for all \( t \in (0, t_{\max}) \).

Theorem 5.4. Let \( \tilde{E} \) be defined in (5.1) and \( \{U^k\} \) be the infinite sequence generated by Algorithm 5.2. Then \( \{U^k\} \) is bounded and has the following property:
\[ \lim_{k \to +\infty} \|\tilde{g}_k\| = 0. \]

Proof. Due to the continuity of \( \tilde{F}, \tilde{G} \) in (5.1) and the coercive property of \( \tilde{F} \), the sublevel set \( \mathcal{M}_0 = \{U : \tilde{E}(U) \leq \tilde{E}(U^0)\} \) is compact for any \( U^0 \). By the inequality (5.8), it is easy to know \( \{E(U^k)\} \) is a decreasing sequence, and thus \( \{U^k\} \subset \mathcal{M}_0 \) and there exists some \( \tilde{E} \) such that \( \tilde{E}(U^k) \to \tilde{E} \) as \( k \to \infty \). Moreover, from (5.10) and \( t_k \in (0, 1] \), we know there exist a compact set \( \mathcal{B}_0 \) such that \( \{U^k + td_k|t \in (0, 1]\} \subset \mathcal{B}_0 \) and thus there exists \( M > 0 \) such that
\[ \|\nabla^2 \tilde{E}(U)\| \leq M, \quad \forall U \in \mathcal{B}_0. \]
From the proof of Lemma 5.3, we know \( M_k \leq M \) for all \( k \). Moreover, there exists some \( \bar{\lambda} > 0 \) such that \( \lambda_{\text{max}}(J_k + \mu_k I) \leq \bar{\lambda} \) for all \( k \). We prove (5.14) by contradiction. Assume \( \limsup_{k \to +\infty} \|\tilde{g}_k\| = \varepsilon > 0 \) and define the index set
\[ \mathcal{I} = \bigcup_{k=1}^{\infty} \mathcal{I}_k := \{j \in \mathbb{N} : j \leq k, \|\tilde{g}_j\| \geq \varepsilon / 2\}. \]
Then, we know \( |\mathcal{I}| = \infty \) where \( |\mathcal{I}| \) denotes the number of the elements of \( \mathcal{I} \). Moreover, for all \( j \in \mathcal{I} \), we know
\[ l_j \geq \varepsilon / 2\bar{\lambda} \quad \text{and} \quad t_{j}^{\max} \geq \bar{t} = \min \left\{ \frac{(1 - \nu)\varepsilon}{M\lambda d^2}, 1 \right\}. \]
Thus, \( \bar{t} \) is a uniform lower bound for the step size \( t \) at \( U^j \) for \( j \in \mathcal{I} \), i.e. \( t_j \geq \bar{t}, \forall j \in \mathcal{I} \), and we have
\[ \tilde{E}(U^0) - \tilde{E}(U^{k+1}) = \sum_{j=0}^{k} (\tilde{E}(U^j) - \tilde{E}(U^{j+1})) \geq \sum_{j \in \mathcal{I}_k} (\tilde{E}(U^j) - \tilde{E}(U^{j+1})) \]
\[ \geq \sum_{j \in \mathcal{I}_k} -\nu t_j \langle \tilde{g}_j, d_j \rangle \geq \frac{\nu \varepsilon}{2\bar{\lambda}} |\mathcal{I}_k|, \]
Let \( k \to \infty \) in (5.18), we know \( \tilde{E}(U^0) - \tilde{E} \geq +\infty \), which leads to a contradiction. \( \square \)
5.3. The Hybrid of AA-BPG and Inexact Newton-PCG methods. The AA-BPG is a first order method while the inexact Newton-PCG method is a second order method, it is natural to mix these two methods to further accelerate the convergence. A key step of mixing two methods is designing a proper criterion to determine when to launch the inexact Newton-PCG method. It is difficult to develop a perfect strategy for all kinds of PFC models. In our experiments, we switch to the Newton type algorithm when the following criteria are met

\[
|E(\hat{\Phi}^k) - E(\hat{\Phi}^{k-1})| < \varepsilon_1 \quad \text{or} \quad \|g_k - g_{k-1}\| < \varepsilon_2,
\]

where \(\varepsilon_1, \varepsilon_2 > 0\). Our proposed hybrid method is summarized in Algorithm 5.3.

Algorithm 5.3 The Hybrid Method

Require: \(\hat{\Phi}^0, \varepsilon_1, \varepsilon_2\);
1: \(k = 0\).
2: while stop criterion is not satisfied do
3: if \(\hat{\Phi}^k\) is good enough for Newton method then
4: Perform inexact Newton-PCG method (Algorithm 5.2);
5: else
6: Perform AA-BPG method (Algorithm 4.1 with \(K = 2\) or \(K = 4\));
7: end if
8: \(k = k + 1\);
9: end while

6. Numerical results. In this section, we present several numerical examples for our proposed methods and compare the efficiency and accuracy with existing methods. Our approaches contain AA-BPG-2 and AA-BPG-4 (see Algorithm 4.1), and hybrid method (see Algorithm 5.2), and the comparison methods [35, 26, 36, 25] include the first-order semi-implicit scheme (SIS), the first-order stabilized semi-implicit scheme (SSIS1), the second-order stabilized semi-implicit scheme (SSIS2), the invariant energy quadrature (IEQ) and scalar auxiliary variable (SAV) approaches. All methods are employed to calculate the stationary states of finite dimensional PFC models, including the LB model for periodic crystals and the LP model for quasicrystals. Note that these methods all guarantee mass conservation. The time steps \(\alpha_k\) in our approaches are obtained adaptively by the linear search technique, while the fixed time steps \(\alpha\) of others are chosen to guarantee the best performance on the premise of energy dissipation. In efficient implementation of the inexact Newton-PCG method, the parameters in (5.6) and (5.7) are set with \(\tau = 0.01\), \(\delta_k = 0.7 \max \Lambda_{b}^{(i)}\), and \(\mu_k\) is chosen as [33]. All experiments were performed on a workstation with a 3.20 GHz CPU (i7-8700, 12 processors). All code were written by MATLAB language without parallel implementation.

6.1. Periodic crystals. For the LB model, we use three dimensional periodic crystals of the double gyroid and the sigma phase, as shown in Figure 1, to demonstrate the performance of our approach. In the hybrid method of Algorithm 5.2, we choose the gradient difference \(\|g_k - g_{k-1}\| < 10^{-3}\) as the measurement to launch the inexact NewtonPCG algorithm.
Fig. 1. The stationary periodic crystals in LB model. (a) Double gyroid phase with \( \xi = 0.1, \tau = -2.0, \gamma = 2.0 \). (b) Sigma phase with \( \xi = 0.1, \tau = 0.01, \gamma = -2.0 \) from two perspectives.

6.1.1. Double gyroid. The double gyroid phase is a continuous network periodic phase whose initial values can be chosen as

\[
\phi(r) = \sum_{h \in \Lambda^0_{DG}} \hat{\phi}(h) e^{i(Bh) \cdot r},
\]

where initial lattice points set \( \Lambda^0_{DG} \subset \mathbb{Z}^3 \) only on which the Fourier coefficients located are nonzero. The corresponding \( \Lambda^0_{DG} \) of the double gyroid phase can be found in the Table 1 in [12]. The double gyroid structure belongs to the cubic crystal system, therefore, the 3-order invertible matrix can be chosen as \( B = \frac{1}{\sqrt{6}}I_3 \). Correspondingly, the computational domain in physical space is \( \Omega = [0, 2\sqrt{6}\pi)^3 \). The parameters in LB model (2.1) are set as \( \xi = 0.1, \tau = -2.0, \gamma = 2.0 \). 128\(^3\) wavefunctions are used in these simulations. Figure 1 (a) shows the stationary solution of double gyroid profile.

Figure 2 gives iteration process of the above-mentioned approaches, including the relative energy difference and the gradient changes with iteration, and the CPU time cost. The reference energy value \( E_s = -12.94291551898271 \) is the finally convergent value. As is evident from these results, our proposed approaches perform more efficiently than the existing methods do for computing the double gyroid structure. The hybrid method is most efficient among these approaches. It has the fastest local convergent speed and costs 4 Newton steps to achieve the error of \( \|g_k\| \) about \( 10^{-12} \). The AA-BPG-4 and AA-BPG-2 approaches have nearly the same numerical behaviors, however, the AA-BPG-4 method spends a little more CPU time than AA-BPG-2 scheme does. The reason is attributed to the cost of solving the subproblem (3.5) at each step. For AA-BPG-2 scheme, (3.5) can be solved analytically, while for AA-BPG-4 method, (3.5) is required to numerically solve a nonlinear system. The SIS, SAV and IEQ approaches have almost the same iterations. Theoretically, the convergence of the SIS is based on the assumption of global Lipschitz constants, while the SAV method always has a modified energy dissipation through adding an arbitrary scaler auxiliary parameter \( C \) which guarantees the boundedness of the bulk energy term. The original energy dissipation property of the SAV method depends on the selection of \( C \). For computing the double gyroid phase, we find that when \( C \) is smaller than \( 10^6 \), the SAV scheme cannot keep the original energy dissipation property even if we adopt a small time step \( \alpha = 0.001 \). Further increasing \( C \) to \( 10^8 \), we can use a large time step \( \alpha = 0.2 \) to obtain the original energy dissipation feature. Note that there exists a gap between the modified energy and the original energy no matter what the auxiliary parameters are. Like in the SAV method, similar results and phenomena have been also found in the IEQ approach. Among the three methods,
EFFICIENT METHODS FOR THE STATIONARY STATES OF PFC MODELS

Fig. 2. Double gyroid phase: comparisons of numerical behaviors of the hybrid method, AA-BPG-2/4 approaches with First row: SIS, SAV and IEQ; Second row: SSIS1 and SSIS2. Left column: Relative energy over iterations; Middle column: Relative energy over CPU times; Right column: Gradient over iterations; The blue and yellow ×s mark where restarts occurred and the magenta o mark where adopts the Newton step.

the SIS spends the fewest CPU times. The reason is that the SAV and IEQ methods requires to solve a subsystem at each step while the SIS does not.

The SSIS1 is an unconditionally stable scheme through imposing a stabilized term on SIS. Its energy law holds under the assumption of the stabilizing parameter greater than the half of global Lipschitz constant. The time step size \( \alpha \) can be arbitrary large while the effective time step size has a limit. From the numerical results, SSIS1 with \( \alpha = 10^4 \) shows a slower convergent rate than the SIS with \( \alpha = 0.2 \) does. An interesting scheme is the conditionally stable SSIS2 proposed in [26] that introduces a center difference stabilizing term to guarantee the second order accuracy. From the point of continuity, the SSIS2 actually adds an inertia term onto the original gradient flow system. The inertia term can accelerate the convergent speed but often accompanied with some oscillations if the time step size is large. As Figure 2 shows, when \( \alpha = 0.1 \) the SSIS2 has almost the same convergent speed with the SSIS1, and holds the energy dissipation property. If increasing \( \alpha \), such as 0.3, the SSIS2 obtains an accelerated speed but with oscillations.

6.1.2. Sigma phase. The second periodic structure considered here is the sigma phase, which is a spherical packed phase recently discovered in block copolymer experiment [15], and the self-consistent mean-field simulation [34]. The sigma phase has a larger, much more complicated tetragonal unit cell with 30 atoms. For such a pattern, we implement our algorithm on bounded computational domain \( \Omega = [0, 27.7884] \times [0, 27.7884] \times [0, 14.1514] \). Correspondingly, the initial values can be found in [34, 1].

When computing the sigma phase, the parameters are set as \( \xi = 1.0, \tau = 0.01, \gamma = 2.0 \) and \( 256 \times 256 \times 128 \) wavefunctions are used to discretize LB energy functional. The stationary morphology is shown in Figure 1 (b). As far as we know, it is the first time to find such complicated sigma phase in such a simple PFC model.

Figure 3 compares our proposed methods with other numerical schemes. We still use the reference energy value \( E_s = -0.93081648457086 \) as the baseline to observe
Fig. 3. Sigma phase: comparisons of numerical behaviors of the hybrid method, AA-BPG-2/4 approaches with other numerical methods. The information of these plots is the same with Figure 2.

the relative energy changes of various numerical approaches. Again, as shown in these results, on the premise of energy dissipation, the new developed approaches demonstrate a better performance over the existing methods in computing the sigma phase. Among these methods, the hybrid method is the most efficient.

6.2. Quasicrystals. For the LP free energy, we take the two dimensional dodecagonal quasicrystal as an example to examine the performance of our proposed approach. For dodecagonal quasicrystals, two length scales $q_1$ and $q_2$ equal to 1 and $2 \cos(\pi/12)$, respectively. Two dimensional dodecagonal quasicrystals can be embedded into four dimensional periodic structures, therefore, the projection method is carried out in four dimensional space. The 4-order invertible matrix $B$ associated with four dimensional periodic structure is chosen as $I_4$. The corresponding computational domain in real space is $[0, 2\pi)^4$. The projection matrix $P$ in Eq. (2.6) of the dodecagonal quasicrystals is

$$(6.2) \quad P = \begin{pmatrix} 1 & \cos(\pi/6) & \cos(\pi/3) & 0 \\ 0 & \sin(\pi/6) & \sin(\pi/3) & 1 \end{pmatrix}.$$ 

The initial solution is

$$(6.3) \quad \phi(r) = \sum_{h \in \Lambda_{0}^{QC}} \hat{\phi}(h)e^{i(\mathcal{P}Bh)^{\top} \cdot r}, \quad r \in \mathbb{R}^2,$$

where initial lattice points set $\Lambda_{0}^{QC} \subset \mathbb{Z}^4$ can be found in the Table 3 in [13] on which the Fourier coefficients $\hat{\phi}(h)$ located are nonzero.

The parameters in LP models are set as $c = 24, \varepsilon = -6, \kappa = 6$, and 384 wavefunctions are used to discretize LP energy functional. The convergent stationary quasicrystal is given in Figure 4, including its order parameter distribution and Fourier spectrum. The numerical behavior of different approaches can be found in Figure 5. To better observe the change tendency, we use the convergent energy value $E_s = -15.974863238156402$ as a baseline to show the relative energy changes against
Efficient methods for the stationary states of PFC models

Fig. 4. The stationary dodecagonal quasicrystal phase in LP model with $c = 2, \varepsilon = -1, \kappa = 2$. Left: physical morphology; Right: Fourier spectral points whose coefficient intensity is larger than 0.01

with iterations. In the hybrid method of Algorithm 5.3, we turn to the NewtonPCG method if energy difference $|E(\hat{\Phi}^k) - E(\hat{\Phi}^{k-1})| < 10^{-4}$. We find again that our proposed approaches are more efficient than others, and the hybrid method has the best performance.

Fig. 5. Dodecagonal quasicrystal: comparisons of numerical behaviors of the hybrid method, AA-BPG-2/4 approaches with other numerical methods. The details of these images are the same with Figure 2.

7. Conclusion. In this paper, efficient and robust computational approaches have been proposed to find the stationary states of PFC models. Instead of formulating the energy minimization as a gradient flow, we applied the modern optimization methods directly on the discretized energy with mass conservation and energy dissipation. Moreover, the AA-BPG method with suitable choice of $h$ overcomes the global Lipschitz constant requirement in theoretical analysis and the time steps are adaptively obtained by line search technique. A hybrid method with the inexact Newton method further accelerates the local convergence of AA-BPG methods. Extensive results in computing periodic crystals and quasicrystals show their advantage in terms of computation efficiency without loss of the accuracy. Thus, it motivate us
to continue finding the deep relationship between the numerical schemes in solving gradient flow and the optimization.

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follows that $S_{\ell} > E$. Proof, we assume that $E$.

Applying Lemma 7.1 for all $k > \ell$ we have a useful lemma for our analysis.

Lemma 7.1 (Uniformized Kurdyka-Lojasiewicz property [5]). Let $\Omega$ be a compact set and $E$ is constant on $\Omega$. Then, there exist $\epsilon > 0, \eta > 0,$ and $\psi \in \Psi_\eta$ such that for all $\bar{u} \in \Omega$ and all $u \in \Gamma_\eta(\bar{u}, \epsilon)$, one has,

$$\psi'(E(u) - E(\bar{u}))\text{dist}(0, \partial E(u)) \geq 1,$$

where $\Psi_\eta = \{\psi \in C[0, \eta] \cap C^1(0, \eta), \psi \text{ is concave, } \psi(0) = 0, \psi' > 0 \text{ on } (0, \eta)\}$ and $\Gamma_\eta(x, \epsilon) = \{y \mid \|x - y\| \leq \epsilon, E(x) < E(y) < E(x) + \eta\}$.

Now, we show the proof of Theorem 3.4, which is similar to the framework in [3].

Proof. Let $S(x^0)$ be the set of limiting points of the sequence $\{x^k\}_{k=0}^\infty$ starting from $x^0$. By the boundedness of $\{x^k\}_{k=0}^\infty$ and the fact $S(x^0) = \cap_{q \in N} \cup_{k \geq q} \{x^k\}$, it follows that $S(x^0)$ is a non-empty and compact set. Moreover, from (3.15), we know $E(x)$ is constant on $S(x^0)$, denoted by $E^*$. If there exists some $k_0$ such that $E(x^{k_0}) = E^*$, then we have $E(x^k) = E^*$ for all $k \geq k_0$ which is from (3.15). In the following proof, we assume that $E(x^k) > E^*$ for all $k$. Therefore, $\forall \epsilon, \eta > 0,$ there exists some $\ell > 0$ such that for all $k > \ell$, we have $\text{dist}(S(x^0), x^k) \leq \epsilon$ and $E^* < E(x^k) < E^* + \eta$, i.e.

$$x \in \Gamma_\eta(x^*, \epsilon) \quad \text{for all } x^* \in S(x^0).$$

Applying Lemma 7.1 for all $k > \ell$ we have

$$\psi'(E(x^k) - E^*)\text{dist}(0, E(x^k)) \geq 1.$$
Form (3.17), it implies
\[
\psi'(E(x^k) - E^*) \geq \frac{1}{c_1(\|x^k - x^{k-1}\| + \bar{w}\|x^{k-1} - x^{k-2}\|)}.
\]
By the convexity of \(\psi\), we have
\[
\psi(E(x^k) - E^*) - \psi(E(x^{k+1}) - E^*) \geq \psi'(E(x^k) - E^*)(E(x^k) - E(x^{k+1})).
\]
Define \(\Delta_{p,q} = \psi(E(x^p) - E^*) - \psi(E(x^q) - E^*)\) and \(C = (1 + \bar{w})c_1/c_0 > 0\). Together with (7.3), (7.4) and (3.15), we have for all \(k > \ell\)
\[
(7.5) \quad \Delta_{k,k+1} \geq \frac{c_0\|x^{k+1} - x^k\|^2}{c_1(\|x^k - x^{k-1}\| + \bar{w}\|x^{k-1} - x^{k-2}\|)} \geq \frac{\|x^{k+1} - x^{k}\|^2}{C(\|x^k - x^{k-1}\| + \|x^{k-1} - x^{k-2}\|)}.
\]
Therefore,
\[
(7.6) \quad 2\|x^{k+1} - x^k\| \leq \frac{1}{2}(\|x^k - x^{k-1}\| + \|x^{k-1} - x^{k-2}\|) + 2C\Delta_{k,k+1},
\]
which is from the geometric inequality. For any \(k > \ell\), summing up (7.6) for \(i = \ell + 1, \ldots, k\), it implies
\[
2 \sum_{i=\ell+1}^{k} \|x^{i+1} - x^i\| \leq \frac{1}{2} \sum_{i=\ell+1}^{k} (\|x^i - x^{i-1}\| + \|x^{i-1} - x^{i-2}\|) + 2C \sum_{i=\ell+1}^{k} \Delta_{i,i+1}
\]
\[
\leq \sum_{i=\ell+1}^{k} (\|x^{i+1} - x^i\| + \|x^{\ell} - x^{\ell-1}\| + \|x^{\ell-1} - x^{\ell-2}\|) + 2C \Delta_{\ell+1,k+1},
\]
where the last inequality is from the fact that \(\Delta_{p,q} + \Delta_{q,r} = \Delta_{p,r}\) for all \(p, q, r \in \mathbb{N}\). Since \(\psi \geq 0\), for any \(k > \ell\) and we have
\[
(7.7) \quad \sum_{i=\ell+1}^{k} \|x^{i+1} - x^i\| \leq \|x^{\ell} - x^{\ell-1}\| + \|x^{\ell-1} - x^{\ell-2}\| + 2C\psi(E(x^\ell) - E^*).
\]
This easily implies that \(\sum_{k=1}^{\infty} \|x^{k+1} - x^k\| < \infty\). Together with Theorem 3.4, we obtain
\[
\lim_{k \to +\infty} x^k = x^*, \quad 0 \in \partial E(x^*).
\]

**Appendix B: Proof of Theorem 3.4.** The proof is similar to the framework in [37]. Let \(x^*\) be the exact solution and \(e_i = x^* - x^i\) for all \(i\). We first prove some important properties of Algorithm 5.1.

**Property I:** \(r_i = Ax^i - b\). From the step 4 of Algorithm 5.1, we have \(\alpha_i Ap_i - 1 = Ax^i - Ax^i - 1\). Then,
\[
\begin{align*}
    r_i &= r_{i-1} + \alpha_i Ap_{i-1} = r_0 + \sum_{j=1}^{i} \alpha_j Ap_{j-1} = -b + \sum_{j=1}^{i} \alpha_j Ap_{j-1} \\
    &= -b + \sum_{j=1}^{i} (Ax^i - Ax^{i-1}) = -b + Ax^i - Ax^0 = Ax^i - b.
\end{align*}
\]
Property II: $\langle p_i, b \rangle = \|r_i\|^2_{M^{-1}}$ ($i = 0, 1, 2, \cdots$). By the formula (5.40) in [21], we know that $\langle r_i, r_j \rangle_{M^{-1}} = 0$ ($i \neq j$). Together with the definition of $\beta_i$ and $p_i$ in Algorithm 5.1, we get

$$\langle p_i, b \rangle = \langle p_i, -r_0 \rangle = \langle M^{-1}r_0, r_0 \rangle = \|r_0\|^2_{M^{-1}},$$

$$\langle p_i, b \rangle = \langle p_i, -r_0 \rangle = \langle M^{-1}r_i, r_0 \rangle + \beta_i\langle p_i, -r_0 \rangle = \beta_i\langle p_i, -r_0 \rangle = \left( \prod_{j=1}^{i} \beta_i \right) \langle p_0, -r_0 \rangle = \left( \prod_{j=1}^{i} \beta_i \right) \|r_0\|^2_{M^{-1}} = \|r_1\|^2_{M^{-1}}, \quad \forall i = 1, 2, \cdots.$$  

Property III: $\|e_i\|_A \geq \|e_{i+1}\|_A$. According to the iteration of $p_i$, on has

$$\langle p_i, -r_{i+1} \rangle = \langle -M^{-1}r_i + \beta_i p_i, -r_{i+1} \rangle = 0 + \beta_i \langle p_i, -r_{i+1} \rangle$$

$$\langle p_i, -r_{i+1} \rangle = \left( \prod_{j=1}^{i} \beta_j \right) \langle p_0, -r_{i+1} \rangle = \left( \prod_{j=1}^{i} \beta_j \right) \langle M^{-1}r_0, r_{i+1} \rangle = 0.$$  

By the property I, we have $Ae_{i+1} = A(x^i - x^{i+1}) = b - Ax^{i+1} = -r_{i+1}$, which implies $\langle p_i, Ae_{i+1} \rangle = 0$. Using the fact that $e_i = e_{i+1} + x^{i+1} - x^i = e_{i+1} + \alpha_{i+1}p_i$, the following equation holds for all $i \geq 0$:

$$\|e_i\|_A^2 = \|e_i + \alpha_{i+1}p_i\|_A^2 = \|e_{i+1}\|_A^2 + 2\alpha_{i+1}\langle p_i, Ae_{i+1} \rangle + \|\alpha_{i+1}p_i\|_A^2$$

$$= \|e_{i+1}\|_A^2 + \alpha_{i+1}^2\|p_{i}\|_A^2 \geq \|e_{i+1}\|_A^2.$$  

Property IV: $\langle x^i, b \rangle \geq \langle x^{i-1}, b \rangle$. The definition of $\alpha_j$ gives $\|r_{j-1}\|^2_{M^{-1}} = \alpha_j\|p_{j-1}\|^2_{A}$. Together with (7.8) and (7.10), we have

$$\langle x^i, b \rangle = \langle x^{i-1}, b \rangle + \langle e_i, b \rangle = \langle x^{i-1}, b \rangle + \sum_{j=0}^{i} \langle \alpha_j p_{j-1}, b \rangle = \sum_{j=1}^{i} \alpha_j \|r_{j-1}\|^2_{M^{-1}}$$

$$= \sum_{j=1}^{i} \alpha_j^2 \|p_{j-1}\|_A^2 = \sum_{j=1}^{i} (\|e_{j-1}\|_A^2 - \|e_{j}\|_A^2) = \|e_0\|_A^2 - \|e_i\|_A^2,$$  

which implies $\langle x^i, b \rangle \geq \langle x^{i-1}, b \rangle$ by the monotonicity of $\|e_i\|_A^2$.

Now, we can prove the main result. By using the definition of $p_0$ and $\alpha_1$, we obtain

$$\frac{\langle x^i, b \rangle}{\|b\|^2} \geq \frac{\langle x^{i+1}, b \rangle}{\|b\|^2} = \frac{\langle x^0 + \alpha_1 p_0, b \rangle}{\|b\|^2} = \alpha_1 \frac{\langle p_0, b \rangle}{\|b\|^2} = \frac{\langle r_0, p_0 \rangle}{\|b\|^2} = \frac{1}{\lambda_{\max}(A)} \lambda_{\max}(M).$$

Since $M$ is positive, we know $M = M^{1/2}M^{1/2}$, where $M^{1/2}$ is still positive. As a result,

$$\|M\| = \lambda_{\max}(M) = \lambda_{\max}(M^{1/2}M^{1/2}) = \lambda_{\max}(M^{1/2}) = \|M^{1/2}\|^2.$$  

Let $y = M^{1/2}p_0$, we get

$$\langle M p_0, p_0 \rangle = \langle y, y \rangle \geq \frac{1}{\lambda_{\text{max}} (M^{-1/2} A M^{-1/2})} = \frac{1}{\lambda_{\text{max}} (A)}.$$  \hfill (7.14)

where the second inequality takes the fact that $\|A B\| \leq \|A\| \cdot \|B\|$. Together with (7.12), we get

$$\langle x_i, b \rangle \geq \langle M p_0, p_0 \rangle \frac{1}{\lambda_{\text{max}} (M)} \geq \frac{1}{\lambda_{\text{max}} (A)} \frac{1}{\lambda_{\text{max}} (A)} = \frac{1}{\lambda_{\text{max}} (A)}.$$ \hfill (7.15)

To verify another inequality, we use (7.11) and the fact that $e_0 = x^* - x^0 = -A^{-1} b$,

$$\frac{\langle x^i, b \rangle}{\|b\|^2} = \frac{\|e_0\|^2_A - \|e_i\|^2_A}{\|b\|^2} \leq \frac{\|e_0\|^2_A}{\|b\|^2} = \frac{\|A^{-1} b\|^2_A}{\|b\|^2} = \frac{\langle b, A^{-1} b \rangle}{\|b\|^2} \leq \frac{1}{\lambda_{\min} (A)}.$$