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Stability and Error Analysis for a C^0 Interior Penalty Method for the Modified Phase Field Crystal Equation

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Abstract
We present a C^0 interior penalty finite element method for the sixth-order modified phase field crystal equation. We demonstrate that the numerical scheme is uniquely solvable, unconditionally energy stable, and convergent. Additionally, the error analysis presented develops a detailed methodology for analyzing time dependent problems utilizing the C^0 interior penalty method. We furthermore support the theory with several numerical experiments.

Keywords Phase field crystal · C^0 interior penalty method · Finite element method · Sixth-order parabolic · Higher-order methods · Nonlinear partial differential equation · Energy stability

1 Introduction

Let $\Omega \subset \mathbb{R}^2$ be an open polygonal domain. In this paper, we present a C^0 interior penalty finite element method for the sixth-order modified phase field crystal (MPFC) equation [1, 32]

$$\partial_{tt}\phi + \beta\,\partial_t\phi = \Delta\left(\phi^3 + \alpha\phi + 2\Delta\phi + \Delta^2\phi\right), \tag{1}$$

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where ϕ is the "atom" density field and $\beta \geq 0$ and $\alpha > 0$ are constants. The MPFC equation was introduced as a novel extension of the phase field crystal (PFC) equation which models the diffusive dynamics in the evolution of ϕ [32]. While the PFC equation has proved to be an efficient tool for addressing crystalline self-organization and pattern formation on the atomic scale [17], it fails to capture the more rapid and instantaneous elastic relaxation: a property crucial in the understanding of the deformation properties of nanocrystalline solids [32].

The MPFC equation can be viewed as a damped wave equation. Another way to describe the MPFC equation is as a pseudo-gradient flow of the dimensionless spacial energy [34]:

$$E(\phi) = \int_{\Omega} \left\{ \frac{1}{4}\phi^4 + \frac{\alpha}{2}\phi^2 - |\nabla \phi|^2 + \frac{1}{2}(\Delta \phi)^2 \right\} dx. \tag{2}$$

Defining the chemical potential as

$$\mu := \delta_{\phi} E = \phi^3 + \alpha\phi + 2\Delta\phi + \Delta^2\phi, \tag{3}$$

with $\delta_{\phi} E$ denoting the variational derivative of E with respect to ϕ, and where either the natural boundary conditions $\partial_n \phi = \partial_n \Delta\phi = \partial_n \mu = 0$ or periodic boundary conditions are assumed, the MPFC equation can be rewritten as

$$\partial_{tt}\phi + \beta\, \partial_t \phi = \Delta\mu. \tag{4}$$

The fast dynamics are captured by the first term on the left-hand side of (4), involving the second-order temporal derivatives, while the slow dynamics are captured in the absence of this term and when $\beta = 1$. The well-posedness of the MPFC equation was presented in [23] along with an analysis of the long-time behavior of solutions and the existence and uniqueness of weak and strong solutions to the MPFC equation was also studied in [33].

Due to the potential impact of the MPFC equation, interest in developing accurate and efficient numerical methods approximating solutions to this equation has grown in recent years. Specifically, Wise et al. developed first order and second order in time finite difference schemes along with multigrid solvers for these schemes in [1, 2] and [34]. Additionally, in [29], Li et al. present several different time marching schemes using the common feature of invariant energy quadratization along with a Fourier spectral spacial discretization. In [27], Guo and Xu present an adaptive time-stepping strategy along with a local discontinuous Galerkin method for the MPFC equation. Furthermore, in [28], Lee et al. present splitting time discretization schemes which also utilize a Fourier spectral spacial discretization. Most recently, Qi and Hou present a Scalar Auxiliary Variable time-stepping strategy along with a finite difference spacial discretization in [31] and Pei, Qi, and Hou present an invariant energy quadratization using a Lagrange multiplier approach in [30]. Finally, in [22], Grasselli and Peirre present a C^0 finite element method where they use splitting techniques in both time and space by introducing two auxiliary variables to obtain a system of four equations.

In contrast, we present and analyze a C^0 interior penalty finite element method for the MPFC equation as was done in a previous paper for the PFC equation [15] that allows us to keep the two equation structure of the MPFC and adopt the time-stepping strategy presented in [1, 2]. The novelty of this paper is twofold. First, this is only the second paper to combine the medius analysis for C^0-IP methods with time dependent problems along with a rigorous error analysis without first showing that solutions to the weak formulation of the PDE satisfies the numerical scheme. It is interesting to note that combining the medius analysis with time-dependent six-order in space PDEs seems to require the invocation of discrete product rules; a strategy not generally utilized in the error analyses of FEMs for parabolic PDEs. It is also interesting to note that the general strategy for the error analysis for a C^0-IP method for the parabolic PFC equation could be extended to achieve an error analysis for the damped wave MPFC equation with only a few adjustments required. This is somewhat surprising and is thanks to the time-stepping strategy that was adopted herein. Second, while the stability and error analyses in this paper and in that of the previously mentioned paper for the PFC equation [15] appear very similar and, indeed, follow a similar structure, one critical difference is that, due to the damped wave equation structure of the MPFC equation, the optimal test function for the fully discrete FEM presented in Sect. 2 is no longer the discrete analog of the chemical potential. Rather, the optimal test function becomes the discrete analog of the inverse Laplacian of the first-order time derivative of the phase field variable.

The C^0-IP method is characterized by the use of C^0 Lagrange finite elements where the C^1 continuity requirement inherent to standard conforming finite element methods has been replaced with interior penalty techniques and was first introduced by Engel et al. [18] and revisited and analyzed by Brenner and colleagues [3–13] also see [19] and [24–26].

The development of the C^0-IP method relies on a weak formulation of (1). To this end, we limit our focus to the case in which natural boundary conditions are assumed and introduce the function space $Z := \{z \in H^2(\Omega) | \mathbf{n} \cdot \nabla z = 0 \text{ on } \partial\Omega\}$. Additionally, we use the standard Sobolev space and norm notation throughout the paper. In particular, we let $\|\cdot\|_{L^p}$ denote the standard L^p norm over the region Ω but specify the notation $\|\cdot\|_{L^p(S)}$ as the L^p norm over a general region $S \subset \mathbb{R}^2$ which is not Ω. Additionally, we rely on the mixed formulation (3)–(4) and, therefore, a weak formulation of (1) may then be written as follows: find (ϕ, μ) such that

$$\phi \in L^\infty(0, T; Z) \cap L^2(0, T; H^3(\Omega)), \tag{5a}$$

$$\partial_{tt}\phi, \partial_t\phi \in L^2(0, T; H_N^{-1}(\Omega)), \tag{5b}$$

$$\mu \in L^2(0, T; H^1(\Omega)), \tag{5c}$$

and there hold for almost all $t \in (0, T)$

$$\langle \partial_{tt}\phi, \nu \rangle + \beta \langle \partial_t\phi, \nu \rangle + (\nabla\mu, \nabla\nu) = 0, \quad \forall\, \nu \in H^1(\Omega), \tag{6a}$$

$$\left((\phi)^3 + \alpha\phi, z\right) - 2(\nabla\phi, \nabla z) + a(\phi, z) - (\mu, z) = 0, \quad \forall\, z \in Z, \tag{6b}$$

with the compatible initial data

$$\partial_t \phi(0) = 0, \quad \text{and} \quad \phi(0) = \phi_0 \in H^4(\Omega) \quad \text{such that } \mathbf{n} \cdot \nabla \phi_0 = 0 \quad \text{and} \quad \mathbf{n} \cdot \nabla \Delta \phi_0 = 0, \quad (7)$$

and where (u, v) is the $L^2(\Omega)$ inner product of u and v and $a(u, v) := \left(\nabla^2 u : \nabla^2 v\right)$ is the inner product of the Hessian matrices of u and v. Additionally, we use the notations $H_N^{-1}(\Omega)$ to indicate the dual space of $H^1(\Omega)$ and $\langle \cdot\,, \cdot \rangle$ to indicate a duality pairing. Throughout the paper, we use the notation $\Phi(t) := \Phi(\cdot\,, t) \in X$, which views a spatiotemporal function as a map from the time interval $[0, T]$ into an appropriate Banach space, X.

The paper proceeds as follows. Section 2 develops the fully discrete C^0 interior penalty finite element method for the phase field crystal model. Section 3 establishes unconditional unique solvability and unconditional stability. Section 4 presents the error analysis. Section 5 demonstrates the effectiveness of our method through two numerical experiments.

2 A C^0 Interior Penalty Finite Element Method

In this section, we develop a fully discrete C^0-IP method for the modified phase field crystal equation (1). Let $\mathscr{T}_h$ be a geometrically conforming, locally quasi-uniform simplicial triangulation of Ω. We introduce the following notation:

- h_K = diameter of triangle K ($h = \max_{K \in \mathscr{T}_h} h_K$),
- v_K = restriction of the function v to the triangle K,
- $|K|$ = area of the triangle K,
- $\mathscr{E}_h$ = the set of the edges of the triangles in $\mathscr{T}_h$,
- e = the edge of a triangle,
- $|e|$ = the length of the edge,
- $Z_h := \{v \in C(\overline{\Omega}) | v_K \in P_2(K) \forall K \in \mathscr{T}_h\}$ the standard Lagrange finite element spaces associated with $\mathscr{T}_h$ of degree 2.

Let M be a positive integer such that $t_m = t_{m-1} + \tau$ for $1 \le m \le M$ where $t_0 = 0$, $t_M = t_F$ with $\tau = {}^{t_F}/_{M}$. With this notation, a fully discrete C^0 interior penalty method for (6) is: given $\phi_h^{m-1} \in Z_h \times Z_h$, find $\left(\phi_h^m, \mu_h^m\right) \in Z_h \times Z_h$ such that for all $\nu_h, z_h \in Z_h$

$$\left(\delta_\tau^2 \phi_h^m, \nu_h\right) + \beta \left(\delta_\tau \phi_h^m, \nu_h\right) + \left(\nabla \mu_h^m, \nabla \nu_h\right) = 0, \quad (8a)$$

$$a_h^{IP}\left(\phi_h^m, z_h\right) + \left(\left(\phi_h^m\right)^3 + \alpha\, \phi_h^m, z_h\right) - 2\left(\nabla \phi_h^{m-1}, \nabla z_h\right) - \left(\mu_h^m, z_h\right) = 0, \quad (8b)$$

where

$$\delta_\tau \phi_h^m := \frac{\phi_h^m - \phi_h^{m-1}}{\tau} \quad \text{and} \quad \delta_\tau^2 \phi_h^m := \frac{\delta_\tau \phi_h^m - \delta_\tau \phi_h^{m-1}}{\tau} = \frac{\phi_h^m - 2\phi_h^{m-1} + \phi_h^{m-2}}{\tau^2}$$

with initial data taken to be $\delta_\tau \phi_h^0 \equiv 0$ ($\phi_h^{-1} \equiv \phi_h^0$), $\phi_h^0 := P_h \phi_0 = P_h \phi(0)$ where $P_h : Z \to Z_h$ is a Ritz projection operator (reminiscent of the projection defined

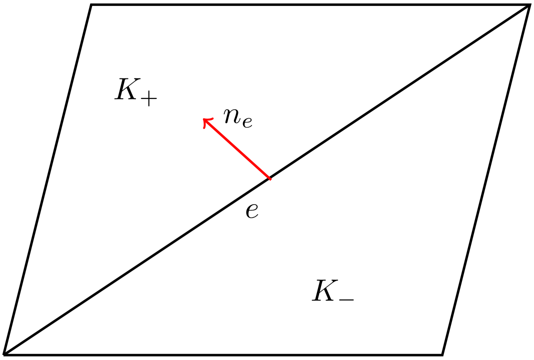

Fig. 1 Orientation of the unit normal n_e outward to the interior triangle K_-. This normal is defined on the interface e shared by the triangles K_- and K_+

in [16, p. 887]) such that

$$a_h^{IP}(P_h\phi - \phi, \xi) + \alpha (P_h\phi - \phi, \xi) = 0 \quad \forall \xi \in Z_h, \quad (P_h\phi - \phi, 1) = 0. \tag{9}$$

The bilinear form $a_h^{IP}(\cdot, \cdot)$ is defined by

$$\begin{aligned} a_h^{IP}(w, v) := & \sum_{K \in \mathscr{T}_h} \int_K \left(\nabla^2 w : \nabla^2 v\right) dx + \sum_{e \in \mathscr{E}_h} \int_e \left\{\!\!\left\{ \frac{\partial^2 w}{\partial n_e^2} \right\}\!\!\right\} \left[\!\!\left[\frac{\partial v}{\partial n_e} \right]\!\!\right] dS \\ & + \sum_{e \in \mathscr{E}_h} \int_e \left\{\!\!\left\{ \frac{\partial^2 v}{\partial n_e^2} \right\}\!\!\right\} \left[\!\!\left[\frac{\partial w}{\partial n_e} \right]\!\!\right] dS + \sigma \sum_{e \in \mathscr{E}_h} \frac{1}{|e|} \int_e \left[\!\!\left[\frac{\partial w}{\partial n_e} \right]\!\!\right] \left[\!\!\left[\frac{\partial v}{\partial n_e} \right]\!\!\right] dS, \end{aligned} \tag{10}$$

with $\sigma \geq 1$ known as a penalty parameter. The jumps and averages that appear in (10) are defined as follows. For an interior edge e shared by two triangles $K_\pm$ where n_e points from K_- to K_+ (see Fig. 1), we define on the edge e

$$\left[\!\!\left[\frac{\partial v}{\partial n_e} \right]\!\!\right] = n_e \cdot (\nabla v_+ - \nabla v_-) \quad \text{and} \quad \left\{\!\!\left\{ \frac{\partial^2 v}{\partial n_e^2} \right\}\!\!\right\} = \frac{1}{2} \left(\frac{\partial^2 v_-}{\partial n_e^2} + \frac{\partial^2 v_+}{\partial n_e^2} \right), \tag{11}$$

where $\dfrac{\partial^2 u}{\partial n_e^2} = n_e \cdot \left(\nabla^2 u\right) n_e$ and where $v_\pm = v|_{K_\pm}$. For a boundary edge e which is an edge of the triangle $K \in \mathscr{T}_h$, we take n_e to be the unit normal pointing towards the outside of Ω and define on the edge e

$$\left[\!\!\left[\frac{\partial v}{\partial n_e} \right]\!\!\right] = -n_e \cdot \nabla v_K \quad \text{and} \quad \left\{\!\!\left\{ \frac{\partial^2 v}{\partial n_e^2} \right\}\!\!\right\} = n_e \cdot \left(\nabla^2 v\right) n_e. \tag{12}$$

Remark 1 Note that the definitions (11) and (12) are independent of the choice of $K_\pm$, or equivalently, independent of the choice of n_e [3].

3 Unique Solvability and Stability

In this section, we show that the C^0-IP method for the MPFC equation outlined in the previous section admits a unique solution and that the system follows an energy law similar to (2). In order to show the existence of a unique solution and unconditional energy stability, we will need the following definitions and lemma. First, we define the following mesh dependent norm

$$\|v_h\|_{2,h}^2 := \sum_{K\in\mathscr{T}_h} |v_h|_{H^2(K)}^2 + \sum_{e\in\mathscr{E}_h} \frac{\sigma}{|e|} \left\| \left[\!\left[\frac{\partial v_h}{\partial n_e} \right]\!\right] \right\|_{L^2(e)}^2, \tag{13}$$

where the seminorm $|w_h|_{H^2(K)}$ is defined by $|w_h|_{H^2(K)}^2 = \int_K \left(\nabla^2 w_h : \nabla^2 w_h\right) dx$. The next lemma guarantees the boundedness of $a_h^{IP}(\cdot,\cdot)$.

Lemma 1 (Boundedness of $a_h^{IP}(\cdot,\cdot)$) *There exists positive constants C_{cont} and C_{coer} such that for choices of the penalty parameter σ large enough we have*

$$a_h^{IP}(w_h, v_h) \le C_{cont}\, \|w_h\|_{2,h}\, \|v_h\|_{2,h} \quad \forall\, w_h, v_h \in Z_h, \tag{14}$$

$$C_{coer}\, \|w_h\|_{2,h}^2 \le a_h^{IP}(w_h, w_h) \quad \forall\, w_h \in Z_h, \tag{15}$$

where the constants C_{cont} and C_{coer} depend only on the shape regularity of $\mathscr{T}_h$.

Proof The proof of the Lemma may be found in [3].

Additionally, we define the spaces $L_0^2(\Omega) := \{v \in L^2(\Omega) | \, (v, 1) = 0\}$, $\mathring{H}^1(\Omega) := H^1(\Omega) \cap L_0^2(\Omega)$, $\mathring{H}_N^{-1}(\Omega) := \{v \in H_N^{-1}(\Omega) | \langle v, 1\rangle = 0\}$, and $\mathring{Z}_h := Z_h \cap L_0^2(\Omega)$. The operator $\mathsf{T} : \mathring{H}_N^{-1}(\Omega) \to \mathring{H}^1(\Omega)$ is often referred to as the 'inverse Laplacian' and is defined via the following variational problem: given $\zeta \in \mathring{H}_N^{-1}(\Omega)$, find $\mathsf{T}\zeta \in \mathring{H}^1(\Omega)$ such that

$$(\nabla \mathsf{T}\zeta, \nabla\chi) = \langle \zeta, \chi\rangle \quad \forall\, \chi \in \mathring{H}^1(\Omega). \tag{16}$$

The well posedness of the operator T is well known, see for example [14], and an induced negative norm may be defined such that $\|v\|_{H_N^{-1}} = (\nabla\mathsf{T}v, \nabla\mathsf{T}v)^{1/2} = \langle v, \mathsf{T}v\rangle^{1/2} = \langle \mathsf{T}v, v\rangle^{1/2}$. We furthermore define a discrete analog of the inverse Laplacian, $\mathsf{T}_h : \mathring{Z}_h \to \mathring{Z}_h$, via the variational problem: given $\zeta \in \mathring{Z}_h$, find $\mathsf{T}_h\zeta \in \mathring{Z}_h$ such that

$$(\nabla \mathsf{T}_h\zeta_h, \nabla\chi_h) = (\zeta_h, \chi_h) \quad \forall\, \chi_h \in \mathring{Z}_h. \tag{17}$$

Again, the well posedness of the operator T_h is well known and a discrete negative inner product and induced norm on $\mathring{Z}_h$ is defined as

$$(v_h, w_h)_{-1,h} := (\nabla\mathsf{T}_h v_h, \nabla\mathsf{T}_h w_h) = (\mathsf{T}_h v_h, w_h) = (v_h, \mathsf{T}_h w_h), \quad \forall v_h, w_h \in \mathring{Z}_h, \tag{18}$$

with

$$\|v_h\|_{-1,h} = (\nabla\mathsf{T}_h v_h, \nabla\mathsf{T}_h v_h)^{1/2}. \tag{19}$$

3.1 Unconditional Unique Solvability and Energy Stability

In this section, we demonstrate that the scheme (8a)–(8b) is unconditionally uniquely solvable and unconditionally energy stable with respect to a modification to the energy (2) for any mesh parameters τ and h and for any of the model parameters such that $\alpha > 0$. To do so, we require the following two lemmas.

Lemma 2 *Assuming solutions to (8) exist and requiring that $\delta_\tau \phi_h^0 = 0$, the scheme (8) satisfies the discrete conservation property $\left(\phi_h^m, 1\right) = \left(\phi_h^0, 1\right) = (P_h \phi_0, 1) = (\phi_0, 1)$ for any $1 \le m \le M$.*

Proof The proof follows similarly to that found in [1].

Remark 2 The quantity $\frac{1}{|\Omega|}(\phi_0, 1)$ is referred to as the average of ϕ_0 over Ω and is denoted by $\overline{\phi}_0$. Due to the discrete conservation property, it follows that $\left(\phi_h^m, 1\right) = \left(\phi_h^0, 1\right) = |\Omega|\, \overline{\phi}_0$.

Lemma 3 *Suppose Ω is a bounded polygonal domain. For all $w_h \in Z_h$, $v \in H^1(\Omega)$, $\gamma > 0$ and σ large enough,*

$$| (\nabla w_h, \nabla v) | \le \sqrt{(1+\gamma)}\, \|w_h\|_{2,h} \, \|v\|_{L^2} \,. \tag{20}$$

Proof See [15].

With these two lemmas in hand, the proof for existence and uniqueness is a two-step process outlined by the following lemma and theorem.

Lemma 4 *Let $\varphi_h^{m-1}, \varphi_h^{m-2}, \in \mathring{Z}_h \times \mathring{Z}_h$ be given. For all $\varphi_h \in \mathring{Z}_h$, define the nonlinear functional*

$$\begin{aligned} G_h(\varphi_h) := \frac{1}{2} \left\| \left(\frac{1+\beta\tau}{\tau^2}\right)^{\frac{1}{2}} \left(\varphi_h - \varphi_h^{m-1}\right) - \left(\frac{1}{\tau^2(1+\beta\tau)}\right)^{\frac{1}{2}} \left(\varphi_h^{m-1} - \varphi_h^{m-2}\right) \right\|_{-1,h}^2 \\ + \frac{1}{2} a_h^{IP}(\varphi_h, \varphi_h) + \frac{1}{4} \left\|\varphi_h + \overline{\phi}_0\right\|_{L^4}^4 + \frac{\alpha}{2} \left\|\varphi_h + \overline{\phi}_0\right\|_{L^2}^2 - 2\left(\nabla \varphi_h^{m-1}, \nabla \varphi_h\right). \end{aligned} \tag{21}$$

The functional G_h is strictly convex and coercive on the linear subspace $\mathring{Z}_h$. Consequently, G_h has a unique minimizer, call it $\varphi_h^m \in \mathring{Z}_h$. Moreover, $\varphi_h^m \in \mathring{Z}_h$ is the unique minimizer of G_h if and only if it is the unique solution to

$$a_h^{IP}\left(\varphi_h^m, z_h\right) + \left(\left(\varphi_h^m + \overline{\phi}_0\right)^3, z_h\right) + \alpha\left(\varphi_h^m + \overline{\phi}_0, z_h\right) - \left(\mu_{h,\star}^m, z_h\right) = 2\left(\nabla \varphi_h^{m-1}, \nabla z_h\right) \tag{22}$$

for all $z_h \in \mathring{Z}_h$, where $\mu_{h,\star}^m \in \mathring{Z}_h$ is the unique solution to

$$\left(\nabla \mu_{h,\star}^m, \nabla \nu_h\right) = -\left(\frac{1+\beta\tau}{\tau^2}\right)\left(\varphi_h^m - \varphi_h^{m-1}, \nu_h\right) + \frac{1}{\tau^2}\left(\varphi_h^{m-1} - \varphi_h^{m-2}, \nu_h\right) \quad \forall \nu_h \in \mathring{Z}_h, \tag{23}$$

with $\varphi_h^{-1} \equiv \varphi_h^0$.

Proof The proof follows those found in [1, 34] with appropriate adjustments relative to the C^0-IP finite element method; similar to those established for the PFC equation found in [15].

Theorem 1 *The scheme* (22)–(23) *is uniquely solvable for any mesh parameters* τ *and* h *and for any* $\alpha > 0$. *Furthermore, the scheme* (22)–(23) *is equivalent to (8). Thus, the scheme (8) is uniquely solvable for any mesh parameters* τ *and* h *and for any* $\alpha > 0$.

Proof The proof follows the approach found in [15].

Energy stability follows as a direct result of the convex decomposition represented in the scheme. First, we define a discrete energy closely related to (2),

$$\mathcal{F}(\phi, \psi) := \frac{1}{4}\|\phi\|_{L^4}^4 + \frac{\alpha}{2}\|\phi\|_{L^2}^2 - \|\nabla\phi\|_{L^2}^2 + \frac{1}{2}a_h^{IP}(\phi, \phi) + \frac{1}{2}\|\psi\|_{-1,h}^2. \quad (24)$$

Lemma 5 *Let* $(\phi_h^m, \mu_h^m) \in Z_h \times Z_h$ *be the solution of* (8a)–(8b). *Then the following energy law holds for any* $h, \tau > 0$ *and for all* $1 \le \ell \le M$:

$$\begin{aligned}
&\mathcal{F}\left(\phi_h^\ell, \delta_\tau\phi_h^\ell\right) + \beta\,\tau\sum_{m=1}^{\ell}\|\delta_\tau\phi_h^m\|_{-1,h}^2 + \frac{1}{2}\sum_{m=1}^{\ell}\left\|\delta_\tau\phi_h^m - \delta_\tau\phi_h^{m-1}\right\|_{-1,h}^2\\
&\quad+\frac{\tau^2}{2}\sum_{m=1}^{\ell}\left(a_h^{IP}\left(\delta_\tau\phi_h^m, \delta_\tau\phi_h^m\right) + \frac{1}{2}\left\|\delta_\tau(\phi_h^m)^2\right\|_{L^2}^2 + \|\phi_h^m\delta_\tau\phi_h^m\|_{L^2}^2 + \alpha\,\|\delta_\tau\phi_h^m\|_{L^2}^2\right.\\
&\quad\left.+2\,\|\nabla\delta_\tau\phi_h^m\|_{L^2}^2\right) = \mathcal{F}\left(\phi_h^0, \delta_\tau\phi_h^0\right).
\end{aligned} \quad (25)$$

Proof Setting $v_h = T_h\delta_\tau\phi_h^m$ in (8a) and $z_h = \delta_\tau\phi_h^m$ in (8b), we have

$$\begin{aligned}
&\left(\delta_\tau^2\phi_h^m, T_h\delta_\tau\phi_h^m\right) + \beta\left(\delta_\tau\phi_h^m, T_h\delta_\tau\phi_h^m\right) + \left(\nabla\mu_h^m, \nabla T_h\delta_\tau\phi_h^m\right) = 0,\\
&a_h^{IP}\left(\phi_h^m, \delta_\tau\phi_h^m\right) + \left(\left(\phi_h^m\right)^3 + \alpha\,\phi_h^m, \delta_\tau\phi_h^m\right) - 2\left(\nabla\phi_h^{m-1}, \nabla\delta_\tau\phi_h^m\right) - \left(\mu_h^m, \delta_\tau\phi_h^m\right) = 0.
\end{aligned}$$

Note that $(\phi_h^m)^3 = 1/2\left[(\phi_h^m)^2\cdot(\phi_h^m - \phi_h^{m-1}) + (\phi_h^m)^2\cdot(\phi_h^m + \phi_h^{m-1})\right]$. Adding the two equations together and using the polarization identity and the definition of the discrete negative norm (19), we obtain

$$\begin{aligned}
&\frac{1}{2\tau}a_h^{IP}\left(\phi_h^m, \phi_h^m\right) - \frac{1}{2\tau}a_h^{IP}\left(\phi_h^{m-1}, \phi_h^{m-1}\right) + \frac{\tau}{2}a_h^{IP}\left(\delta_\tau\phi_h^m, \delta_\tau\phi_h^m\right)\\
&\quad+\frac{1}{4\tau}\left(\|\phi_h^m\|_{L^4}^4 - \left\|\phi_h^{m-1}\right\|_{L^4}^4\right) + \frac{\tau}{4}\|\delta_\tau(\phi_h^m)^2\|_{L^2}^2 + \frac{\tau}{2}\|\phi_h^m\delta_\tau\phi_h^m\|_{L^2}^2\\
&\quad+\frac{\alpha}{2\tau}\left(\|\phi_h^m\|_{L^2}^2 - \left\|\phi_h^{m-1}\right\|_{L^2}^2\right) + \frac{\alpha\tau}{2}\|\delta_\tau\phi_h^m\|_{L^2}^2 - \frac{1}{\tau}\left(\|\nabla\phi_h^m\|_{L^2}^2 - \left\|\nabla\phi_h^{m-1}\right\|_{L^2}^2\right)\\
&\quad+\tau\,\|\nabla\delta_\tau\phi_h^m\|_{L^2}^2 + \beta\,\|\delta_\tau\phi_h^m\|_{-1,h}^2\\
&\quad+\frac{1}{2\tau}\left(\|\delta_\tau\phi_h^m\|_{-1,h}^2 - \left\|\delta_\tau\phi_h^{m-1}\right\|_{-1,h}^2 + \left\|\delta_\tau\phi_h^m - \delta_\tau\phi_h^{m-1}\right\|_{-1,h}^2\right) = 0.
\end{aligned}$$

Applying $\tau \sum_{m=1}^{\ell}$ yields the desired result.

The discrete energy law immediately implies the following uniform *a priori* estimates for ϕ_h^m and $\delta_\tau \phi_h^m$.

Lemma 6 *Let* $(\phi_h^m, \mu_h^m) \in Z_h \times Z_h$ *be the unique solution of* (8a)–(8b). *Suppose that* $\mathcal{F}(\phi_h^0, \delta_\tau \phi_h^0) \leq C$, *where* C *is independent of* h, *and that* $\alpha > \frac{(1+\gamma)}{C_{coer}} - 1 > 0$. *Then the following estimates hold for any* $\tau, h > 0$ *and any* $1 \leq \ell \leq M$:

$$\max_{0\leq\ell\leq M}\left[\left\|\phi_h^\ell\right\|_{L^4}^4 + \left\|\phi_h^\ell\right\|_{L^2}^2 + \left\|\phi_h^\ell\right\|_{H^1}^2 + \left\|\phi_h^\ell\right\|_{2,h}^2 + \left\|\delta_\tau \phi_h^\ell\right\|_{-1,h}^2\right] \leq C, \tag{26}$$

$$\tau \sum_{m=1}^{\ell} \left\|\delta_\tau \phi_h^m\right\|_{-1,h}^2 \leq C, \tag{27}$$

$$\tau^2 \sum_{m=1}^{\ell}\left\{ \left\|\delta_\tau \phi_h^m\right\|_{H^1}^2 + \left\|\phi_h^m \delta_\tau \phi_h^m\right\|_{L^2}^2 + \left\|\delta_\tau \phi_h^m\right\|_{2,h}^2 \right\} \leq C, \tag{28}$$

for some constant C *that is independent of* h, τ, *and* T.

Proof The proof follows as a result of Lemmas 3 and 5. More specifically, Lemma 5 yields, for any $1 \leq m \leq M$,

$$\frac{1}{4}\left\|\phi_h^m\right\|_{L^4}^4 + \frac{\alpha}{2}\left\|\phi_h^m\right\|_{L^2}^2 - \left\|\nabla\phi_h^m\right\|_{L^2}^2 + \frac{1}{2}a_h^{IP}\left(\phi_h^m, \phi_h^m\right) + \frac{1}{2}\left\|\delta_\tau \phi_h^m\right\|_{-1,h}^2 \leq C_0,$$

where $C_0 := \frac{1}{4}\left\|\phi_h^0\right\|_{L^4}^4 + \frac{\alpha}{2}\left\|\phi_h^0\right\|_{L^2}^2 - \left\|\nabla\phi_h^0\right\|_{L^2}^2 + \frac{1}{2}a_h^{IP}\left(\phi_h^0, \phi_h^0\right) + \frac{1}{2}\left\|\delta_\tau \phi_h^0\right\|_{-1,h}^2$. Multiplying by 2, invoking Lemma 3, Young's inequality, and (15), we have

$$\begin{aligned}
\frac{1}{2}\left\|\phi_h^m\right\|_{L^4}^4 + \alpha\left\|\phi_h^m\right\|_{L^2}^2 + C_{coer}\left\|\phi_h^m\right\|_{2,h}^2 + \left\|\delta_\tau \phi_h^m\right\|_{-1,h}^2 &\leq C_0 + 2\left\|\nabla\phi_h^m\right\|_{L^2}^2 \\
&\leq C_0 + 2\sqrt{(1+\gamma)}\left\|\phi_h^m\right\|_{2,h}\left\|\phi_h^m\right\|_{L^2} \\
&\leq C_0 + C_{coer}\left\|\phi_h^m\right\|_{2,h}^2 + \frac{(1+\gamma)}{C_{coer}}\left\|\phi_h^m\right\|_{L^2}^2.
\end{aligned}$$

Now using the fact that $0 < (u^2-1)^2 = u^4 - 2u^2 + 1$ implies that $\frac{1}{2}\left\|\phi_h^m\right\|_{L^4}^4 > \left\|\phi_h^m\right\|_{L^2}^2 - \frac{1}{2}|\Omega|$, where $|\Omega|$ indicates the volume of Ω, we have

$$\begin{aligned}
(\alpha+1)\left\|\phi_h^m\right\|_{L^2}^2 + C_{coer}\left\|\phi_h^m\right\|_{2,h}^2 + \left\|\delta_\tau \phi_h^m\right\|_{-1,h}^2 &\leq C_0 + 2\left\|\nabla\phi_h^m\right\|_{L^2}^2 \\
&\leq C_0 + C_{coer}\left\|\phi_h^m\right\|_{2,h}^2 + \frac{(1+\gamma)}{C_{coer}}\left\|\phi_h^m\right\|_{L^2}^2 + \frac{1}{2}|\Omega|.
\end{aligned}$$

Combining like terms and dropping several of the resulting positive terms on the left-hand side of the equation, we have

$$\left(\alpha + 1 - \frac{(1+\gamma)}{C_{coer}}\right)\left\|\phi_h^m\right\|_{L^2}^2 \leq C_0 + \frac{1}{2}|\Omega| = C.$$

This gives the estimate for $\left\|\phi_h^m\right\|_{L^2}^2$ by requiring that $\alpha > \frac{(1+\gamma)}{C_{coer}} - 1 > 0$. The remaining estimates are obtained as follows:

$$\begin{aligned}\frac{1}{2}\left\|\phi_h^m\right\|_{L^4}^4 + \alpha\left\|\phi_h^m\right\|_{L^2}^2 + C_{coer}\left\|\phi_h^m\right\|_{2,h}^2 + \left\|\delta_\tau\phi_h^m\right\|_{-1,h}^2 &\le C_0 + 2\left\|\nabla\phi_h^m\right\|_{L^2}^2 \\ &\le C_0 + 2\sqrt{(1+\gamma)}\left\|\phi_h^m\right\|_{2,h}\left\|\phi_h^m\right\|_{L^2} \\ &\le C_0 + \frac{C_{coer}}{2}\left\|\phi_h^m\right\|_{2,h}^2 + \frac{2(1+\gamma)}{C_{coer}}\left\|\phi_h^m\right\|_{L^2}^2.\end{aligned}$$

Combining like terms and invoking the bound above, we have

$$\frac{1}{2}\left\|\phi_h^m\right\|_{L^4}^4 + \alpha\left\|\phi_h^m\right\|_{L^2}^2 + \frac{C_{coer}}{2}\left\|\phi_h^m\right\|_{2,h}^2 + \left\|\delta_\tau\phi_h^m\right\|_{-1,h}^2 \le C.$$

Remark 3 Following [3], we note that C_{coer} can be chosen to be close to 1 as long as the penalty parameter σ is large enough. In this case, γ could also be chosen close to 0 and Lemma 6 will hold as long as $\alpha > 0$.

4 Error Estimates

In this section, we provide a rigorous convergence analysis for the fully-discrete method in the appropriate energy norms. We shall assume that the weak solutions have the additional regularities

$$\begin{aligned}\phi &\in L^\infty\left(0,T;H^3(\Omega)\right) \cap L^2\left(0,T;H^3(\Omega)\right),\\ \partial_t\phi &\in L^2\left(0,T;H^3(\Omega)\right) \cap L^2(0,T;H_N^{-1}(\Omega)),\\ \partial_{tt}\phi &\in L^2\left(0,T;L^2(\Omega)\right),\\ \mu &\in L^2\left(0,T;H^2(\Omega)\right),\\ \partial_t\mu &\in L^2\left(0,T;L^2(\Omega)\right).\end{aligned} \tag{29}$$

Such solutions have been shown to exist by Wang and Wise [33].

The interior penalty method (8a)–(8b) is not well-defined for solutions to (6) since $Z_h \not\subset Z$. Therefore, we define $W_h \subset Z$ to be the Hsieh–Clough–Tocher micro finite element space associated with $\mathscr{T}_h$ as in [4]. We furthermore define the linear map $E_h : Z_h \to W_h \cap Z$ as in [4] which allows us to consider the following problem: find $(\phi,\mu) \in Z \times H^1(\Omega)$ such that

$$(\partial_{tt}\phi, \nu_h) + \beta\,(\partial_t\phi, \nu_h) + (\nabla\mu, \nabla\nu_h) = 0, \quad \forall\, \nu_h \in Z_h, \tag{30a}$$

$$a(\phi, E_h z_h) + \left((\phi)^3 + \alpha\phi, E_h z_h\right) - 2\,(\nabla\phi, \nabla E_h z_h) - (\mu, E_h z_h) = 0 \quad \forall\, z_h \in Z_h. \tag{30b}$$

Now, adding and subtracting appropriate terms and using the fact that $a_h^{IP}(\phi, E_h\psi) = a(\phi, E_h\psi)$ for all $\psi \in Z_h$, we obtain a system with solutions that are consistent with those of solutions of (31): find $(\phi, \mu) \in Z \times H^1(\Omega)$ such that

$$(\partial_{tt}\phi, v_h) + \beta\ (\partial_t\phi, v_h) + (\nabla\mu, \nabla v_h) = 0, \quad \forall\, v_h \in Z_h, \tag{31a}$$

$$\begin{aligned} &a_h^{IP}(\phi, z_h) + \left((\phi)^3 + \alpha\phi, z_h\right) - 2\,(\nabla\phi, \nabla z_h) - (\mu, z_h) \\ &\quad = a_h^{IP}(\phi, z_h - E_h z_h) + \left((\phi)^3 + \alpha\phi, z_h - E_h z_h\right) \\ &\qquad - 2\,(\nabla\phi, \nabla z_h - \nabla E_h z_h) - (\mu, z_h - E_h z_h)\,, \quad \forall\, z_h \in Z_h. \end{aligned} \tag{31b}$$

Remark 4 One of the primary challenges in the error analysis to follow arises due to insufficient global regularity possessed by solutions to (6) in the space Z_h. To remedy this, we rely on considering the Hsieh–Clough–Tocher micro finite element space associated with $\mathscr{T}_h$ with the help of the enriching operator $E_h : Z_h \to W_h \cap Z$ as stated above. The analysis to follow employs a combination of essentially standard techniques for conforming time dependent finite element methods and a medius analysis for C^0-IP methods. If one wanted to avoid the medius analysis, then one would need to show that solutions to (6) satisfy the numerical scheme as is done in [24] for the extended Fisher–Kolmogorov equation. It is unclear whether or not this could be achieved for the MPFC equation and is reserved for future work.

Additionally, we introduce the following notation:

$$\begin{aligned} \mathbb{e}^{\phi,m} &= \mathbb{e}_P^{\phi,m} + \mathbb{e}_h^{\phi,m}, \quad \mathbb{e}_P^{\phi,m} := \phi^m - P_h\phi^m, \quad \mathbb{e}_h^{\phi,m} := P_h\phi^m - \phi_h^m, \\ \mathbb{e}^{\mu,m} &= \mathbb{e}_R^{\mu,m} + \mathbb{e}_h^{\mu,m}, \quad \mathbb{e}_R^{\mu,m} := \mu^m - R_h\mu^m, \quad \mathbb{e}_h^{\mu,m} := R_h\mu^m - \mu_h^m, \end{aligned}$$

where $\phi^m := \phi(t_m)$ and $R_h : H^1(\Omega) \to Z_h$ is a Ritz projection operator such that

$$(\nabla(R_h\mu - \mu), \nabla\xi) = 0, \quad \forall\, \xi \in Z_h, \quad (R_h\mu - \mu, 1) = 0. \tag{32}$$

Using this notation and subtracting (8) from (31), we have for all $v_h \in Z_h$ and $z_h \in Z_h$

$$\begin{aligned} &\left(\delta_\tau^2 \mathbb{e}^{\phi,m}, v_h\right) + \beta\ \left(\delta_\tau \mathbb{e}^{\phi,m}, v_h\right) + \left(\nabla\mathbb{e}^{\mu,m}, \nabla v_h\right) \\ &\quad = \left(\delta_\tau^2\phi^m - \partial_{tt}\phi^m, v_h\right) + \beta\ \left(\delta_\tau\phi^m - \partial_t\phi^m, v_h\right), \end{aligned}$$

$$\begin{aligned} &a_h^{IP}\left(\mathbb{e}^{\phi,m}, z_h\right) + \alpha\ \left(\mathbb{e}^{\phi,m}, z_h\right) - 2\left(\nabla\mathbb{e}^{\phi,m-1}, \nabla z_h\right) - \left(\mathbb{e}^{\mu,m}, z_h\right) \\ &\quad = -\left(\left(\phi^m\right)^3 - \left(\phi_h^m\right)^3, z_h\right) - 2\left(\nabla\phi^{m-1} - \nabla\phi^m, \nabla z_h\right) + a_h^{IP}\left(\phi^m, z_h - E_h z_h\right) \\ &\qquad + \left(\left(\phi^m\right)^3 + \alpha\phi^m, z_h - E_h z_h\right) - 2\left(\nabla\phi^m, \nabla z_h - \nabla E_h z_h\right) - \left(\mu^m, z_h - E_h z_h\right). \end{aligned}$$

Invoking the properties of the projection operators, we have for all $\nu_h \in Z_h$ and all $z_h \in Z_h$,

$$\frac{1}{\tau}\left(\delta_\tau \mathbb{e}_h^{\phi,m} - \delta_\tau \mathbb{e}_h^{\phi,m-1}, \nu_h\right) + \beta\left(\delta_\tau \mathbb{e}_h^{\phi,m}, \nu_h\right) + \left(\nabla \mathbb{e}_h^{\mu,m}, \nabla \nu_h\right)$$
$$= \left(\delta_\tau^2 \phi^m - \partial_{tt}\phi^m, \nu_h\right) + \beta\left(\delta_\tau \phi^m - \partial_t \phi^m, \nu_h\right)$$
$$- \frac{1}{\tau}\left(\delta_\tau \mathbb{e}_P^{\phi,m} - \delta_\tau \mathbb{e}_P^{\phi,m-1}, \nu_h\right) - \beta\left(\delta_\tau \mathbb{e}_P^{\phi,m}, \nu_h\right), \tag{33}$$

$$a_h^{IP}\left(\mathbb{e}_h^{\phi,m}, z_h\right) + \alpha\left(\mathbb{e}_h^{\phi,m}, z_h\right) - 2\left(\nabla \mathbb{e}_h^{\phi,m-1}, \nabla z_h\right) - \left(\mathbb{e}_h^{\mu,m}, z_h\right)$$
$$= 2\left(\nabla \mathbb{e}_P^{\phi,m-1}, \nabla z_h\right) + \left(\mathbb{e}_R^{\mu,m}, z_h\right) - \left(\left(\phi^m\right)^3 - \left(\phi_h^m\right)^3, z_h\right) - 2\left(\nabla\phi^{m-1} - \nabla\phi^m, \nabla z_h\right)$$
$$+ a_h^{IP}\left(\phi^m, z_h - E_h z_h\right) + \left(\left(\phi^m\right)^3 + \alpha\phi^m, z_h - E_h z_h\right)$$
$$- 2\left(\nabla\phi^m, \nabla z_h - \nabla E_h z_h\right) - \left(\mu^m, z_h - E_h z_h\right). \tag{34}$$

Setting $\nu_h = T_h \delta_\tau \mathbb{e}_h^{\phi,m}$ and $z_h = \delta_\tau \mathbb{e}_h^{\phi,m}$ and adding and subtracting $4\left(\mathbb{e}_h^{\phi,m}, \delta_\tau \mathbb{e}_h^{\phi,m}\right)$, we arrive at the key error equation

$$\beta\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2 + \frac{1}{\tau}\left(\delta_\tau \mathbb{e}_h^{\phi,m} - \delta_\tau \mathbb{e}_h^{\phi,m-1}, T_h \delta_\tau \mathbb{e}_h^{\phi,m}\right) + a_h^{IP}\left(\mathbb{e}_h^{\phi,m}, \delta_\tau \mathbb{e}_h^{\phi,m}\right)$$
$$+ \alpha\left(\mathbb{e}_h^{\phi,m}, \delta_\tau \mathbb{e}_h^{\phi,m}\right) + 4\left(\mathbb{e}_h^{\phi,m}, \delta_\tau \mathbb{e}_h^{\phi,m}\right) - 2\left(\nabla \mathbb{e}_h^{\phi,m-1}, \nabla \delta_\tau \mathbb{e}_h^{\phi,m}\right)$$
$$= \left(\delta_\tau^2 \phi^m - \partial_{tt}\phi^m, T_h \delta_\tau \mathbb{e}_h^{\phi,m}\right) + \beta\left(\delta_\tau \phi^m - \partial_t \phi^m, T_h \delta_\tau \mathbb{e}_h^{\phi,m}\right)$$
$$- \frac{1}{\tau}\left(\delta_\tau \mathbb{e}_P^{\phi,m} - \delta_\tau \mathbb{e}_P^{\phi,m-1}, T_h \delta_\tau \mathbb{e}_h^{\phi,m}\right) - \beta\left(\delta_\tau \mathbb{e}_P^{\phi,m}, T_h \delta_\tau \mathbb{e}_h^{\phi,m}\right)$$
$$+ 4\left(\mathbb{e}_h^{\phi,m}, \delta_\tau \mathbb{e}_h^{\phi,m}\right) + 2\left(\nabla \mathbb{e}_P^{\phi,m-1}, \nabla \delta_\tau \mathbb{e}_h^{\phi,m}\right) + \left(\mathbb{e}_R^{\mu,m}, \delta_\tau \mathbb{e}_h^{\phi,m}\right)$$
$$- \left(\left(\phi^m\right)^3 - \left(\phi_h^m\right)^3, \delta_\tau \mathbb{e}_h^{\phi,m}\right) + 2\left(\nabla\phi^m - \nabla\phi^{m-1}, \nabla \delta_\tau \mathbb{e}_h^{\phi,m}\right)$$
$$+ a_h^{IP}\left(\phi^m, \delta_\tau \mathbb{e}_h^{\phi,m} - E_h \delta_\tau \mathbb{e}_h^{\phi,m}\right) + \left(\left(\phi^m\right)^3 + \alpha\phi^m, \delta_\tau \mathbb{e}_h^{\phi,m} - E_h \delta_\tau \mathbb{e}_h^{\phi,m}\right)$$
$$- 2\left(\nabla\phi^m, \nabla \delta_\tau \mathbb{e}_h^{\phi,m} - \nabla E_h \delta_\tau \mathbb{e}_h^{\phi,m}\right) - \left(\mu^m, \delta_\tau \mathbb{e}_h^{\phi,m} - E_h \delta_\tau \mathbb{e}_h^{\phi,m}\right). \tag{35}$$

The following lemma will bound many of the terms on the right hand side of (35) by oscillations in the chemical potential μ which is considered data. The procedure is known as a medius analysis and has been utilized in much of the literature found on the C^0-IP method and details can be found in [3].

Lemma 7 *Suppose* (ϕ^m, μ^m) *is a weak solution to (6), with the additional regularities* (29). *Then for any* $h, \tau > 0$ *and any* $1 \leq m \leq M$,

$$a_h^{IP}\left(\phi^m, \mathbb{e}_h^{\phi,m} - E_h \mathbb{e}_h^{\phi,m}\right) + \left(\left(\phi^m\right)^3 + \alpha\phi^m, \mathbb{e}_h^{\phi,m} - E_h \mathbb{e}_h^{\phi,m}\right)$$
$$- 2\left(\nabla\phi^m, \nabla\left(\mathbb{e}_h^{\phi,m} - E_h \mathbb{e}_h^{\phi,m}\right)\right) - \left(\mu^m, \mathbb{e}_h^{\phi,m} - E_h \mathbb{e}_h^{\phi,m}\right)$$

$$\leq C\left[Osc_j(\mu^m)\right]^2 + C\left\|\mathbb{e}_P^{\phi,m}\right\|_{2,h}^2 + \frac{C_{coer}}{4\kappa}\left\|\mathbb{e}_h^{\phi,m}\right\|_{2,h}^2, \tag{36}$$

and

$$\begin{aligned} a_h^{IP}&\left(\delta_\tau\phi^m, \mathbb{e}_h^{\phi,m-1} - E_h\mathbb{e}_h^{\phi,m-1}\right) + \left(\delta_\tau\left((\phi^m)^3 + \alpha\phi^m\right), \mathbb{e}_h^{\phi,m-1} - E_h\mathbb{e}_h^{\phi,m-1}\right) \\ &- 2\left(\delta_\tau\nabla\phi^m, \nabla\left(\mathbb{e}_h^{\phi,m-1} - E_h\mathbb{e}_h^{\phi,m-1}\right)\right) - \left(\delta_\tau\mu^m, \mathbb{e}_h^{\phi,m-1} - E_h\mathbb{e}_h^{\phi,m-1}\right) \\ &\leq C\left[Osc_j(\partial_t\mu(t^*))\right]^2 + C\left\|\mathbb{e}_P^{\phi,m}\right\|_{2,h}^2 + C\left\|\mathbb{e}_h^{\phi,m-1}\right\|_{2,h}^2, \end{aligned} \tag{37}$$

for $t^* \in (t_m, t_{m+1})$, where the arbitrary constant $\kappa > 0$ and where $Osc_j(\nu)$ is referred to as the oscillation of ν (of order j) defined by

$$Osc_j(\nu) := \left(\sum_{K\in\mathscr{T}_h} h^4\left\|\nu - \tilde{\nu}\right\|_{L^2(K)}^2\right)^{\frac{1}{2}}. \tag{38}$$

Here, $\tilde{\nu}$ is the L^2 orthogonal projection of ν on $P_j(\Omega, \mathscr{T}_h)$, the space of piecewise polynomial functions of degree less than or equal to j, i.e.,

$$\int_\Omega(\nu - \tilde{\nu})\psi\, dx = 0 \quad \forall\psi \in P_j(\Omega, \mathscr{T}_h).$$

Proof See [15].

We are now in position to prove the main theorem in this section.

Theorem 2 *Suppose (ϕ^m, μ^m) is a weak solution to (6), with the additional regularities (29). Then for any $h > 0$, $0 < \tau < \tau_0$, $\alpha > \max\left\{\frac{(1+\gamma)}{C_{coer}} - 1, \frac{4(1+\gamma)}{C_{coer}} - 4\right\} > 0$ with τ_0 sufficiently small and any $1 \leq \ell \leq M$,*

$$\begin{aligned} &\left\|\mathbb{e}_h^{\phi,\ell}\right\|_{2,h}^2 + C\left\|\mathbb{e}_h^{\phi,\ell}\right\|_{L^2}^2 + C\tau\sum_{m=1}^{\ell}\left\|\mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2 \\ &\quad + C\tau^2\sum_{m=1}^{\ell}\left[\left\|\delta_\tau\mathbb{e}_h^{\phi,\ell}\right\|_{2,h}^2 + \alpha\left\|\delta_\tau\mathbb{e}_h^{\phi,m}\right\|_{L^2}^2 + \left\|\nabla\delta_\tau\mathbb{e}_h^{\phi,m}\right\|_{L^2}^2\right] \leq C^*(h^2 + \tau^2), \end{aligned} \tag{39}$$

where C^* may depend on the oscillations of μ and $\partial_t\mu$ and the final stopping time T but does not depend upon the spacial step size h or the time step size τ.

Proof First, we note that for all $\chi \in Z_h$ and all $\zeta \in \mathring{Z}_h$ [14],

$$|(\zeta, \chi)| \leq \|\zeta\|_{-1,h}\|\nabla\chi\|_{L^2} \tag{40}$$

and similarly for all $g \in Z$ and all $\zeta \in \mathring{Z}_h$,

$$|(\zeta, g)| \leq \|\zeta\|_{-1,h} \|\nabla g\|_{L^2}. \tag{41}$$

Starting with the first five terms on the right hand side of (35) and using Young's and Hölder's inequalities, Poincaré's inequality, Taylor's theorem, and properties (40) and (41), we have

$$\begin{aligned}
\left(\delta_\tau^2 \phi^m - \partial_{tt}\phi^m, T_h\delta_\tau \mathbb{e}_h^{\phi,m}\right) &= \left(\frac{\phi^m - 2\phi^{m-1} + \phi^{m-2}}{\tau^2} - \partial_{tt}\phi^m, T_h\delta_\tau \mathbb{e}_h^{\phi,m}\right) \\
&\leq \left\|\frac{\phi^m - 2\phi^{m-1} + \phi^{m-2}}{\tau^2} - \partial_{tt}\phi^m\right\|_{L^2} \left\|T_h\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{L^2} \\
&\leq C\tau \int_{t_{m-2}}^{t_m} \|\partial_{sss}\phi(s)\|_{L^2}^2\, ds + \frac{\beta}{16}\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2, \qquad (42)\\
\beta\left(\delta_\tau\phi^m - \partial_t\phi^m, T_h\delta_\tau \mathbb{e}_h^{\phi,m}\right) &\leq \beta\left\|\delta_\tau\phi_h^m - \partial_t\phi^m\right\|_{L^2}\left\|T_h\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{L^2} \\
&\leq C\tau \int_{t_{m-1}}^{t_m} \|\partial_{ss}\phi(s)\|_{L^2}^2\, ds + \frac{\beta}{16}\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2, \qquad (43)\\
-\frac{1}{\tau}\left(\delta_\tau \mathbb{e}_P^{\phi,m} - \delta_\tau \mathbb{e}_P^{\phi,m-1}, T_h\delta_\tau \mathbb{e}_h^{\phi,m}\right) &\leq \left\|\frac{\delta_\tau \mathbb{e}_P^{\phi,m} - \delta_\tau \mathbb{e}_P^{\phi,m-1}}{\tau}\right\|_{L^2}\left\|T_h\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{L^2} \\
&\leq C\left\|\frac{\delta_\tau \mathbb{e}_P^{\phi,m} - \delta_\tau \mathbb{e}_P^{\phi,m-1}}{\tau}\right\|_{L^2}^2 + \frac{\beta}{16}\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2 \\
&\leq \frac{C}{\tau}\int_{t_{m-2}}^{t_m} \|P_h\partial_{ss}\phi(s) - \partial_{ss}\phi(s)\|_{L^2}^2\, ds + \frac{\beta}{16}\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2 \\
&\leq \frac{C}{\tau}\int_{t_{m-2}}^{t_m} \|\partial_{ss}\phi(s) - P_h\partial_{ss}\phi(s)\|_{2,h}^2\, ds + \frac{\beta}{16}\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2, \qquad (44)\\
-\beta\left(\delta_\tau \mathbb{e}_P^{\phi,m}, T_h\delta_\tau \mathbb{e}_h^{\phi,m}\right) &\leq \beta\left\|\delta_\tau \mathbb{e}_P^{\phi,m}\right\|_{L^2}\left\|T_h\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{L^2} \\
&\leq C\left\|\delta_\tau \mathbb{e}_P^{\phi,m}\right\|_{L^2}^2 + \frac{\beta}{16}\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2 \\
&\leq \frac{C}{\tau}\int_{t_{m-1}}^{t_m} \|P_h\partial_s\phi(s) - \partial_s\phi(s)\|_{L^2}^2\, ds + \frac{\beta}{16}\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2 \\
&\leq \frac{C}{\tau}\int_{t_{m-1}}^{t_m} \|\partial_s\phi(s) - P_h\partial_s\phi(s)\|_{2,h}^2\, ds + \frac{\beta}{16}\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2, \qquad (45)
\end{aligned}$$

and

$$4\left(\mathbb{e}_h^{\phi,m}, \delta_\tau \mathbb{e}_h^{\phi,m}\right) \leq C\left\|\mathbb{e}_h^{\phi,m}\right\|_{2,h}^2 + \frac{\beta}{16}\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2. \tag{46}$$

We note that inequalities (42) and (44) above holds for all $m \geq 2$. For $m = 1$, the inequalities becomes

$$\left(\frac{\phi^1-\phi^0}{\tau^2}-\partial_{tt}\phi^1, T_h\delta_\tau \mathbb{e}_h^{\phi,1}\right) \le \left\|\frac{\phi^1-\phi^0}{\tau^2}-\partial_{tt}\phi^1\right\|_{L^2}\left\|T_h\delta_\tau \mathbb{e}_h^{\phi,1}\right\|_{L^2}$$
$$\le C\tau\int_{t_0}^{t_1}\|\partial_{ss}\phi(s)\|_{L^2}^2+\|\partial_{sss}\phi(s)\|_{L^2}^2\,ds+\frac{\beta}{16}\left\|\delta_\tau \mathbb{e}_h^{\phi,1}\right\|_{-1,h}^2,$$

and

$$-\frac{1}{\tau}\left(\delta_\tau \mathbb{e}_P^{\phi,1}, T_h\delta_\tau \mathbb{e}_h^{\phi,1}\right) \le \left\|\frac{\delta_\tau \mathbb{e}_P^{\phi,1}}{\tau}\right\|_{L^2}\left\|T_h\delta_\tau \mathbb{e}_h^{\phi,1}\right\|_{L^2}$$
$$\le C\left\|\frac{\delta_\tau \mathbb{e}_P^{\phi,1}}{\tau}\right\|_{L^2}^2+\frac{\beta}{16}\left\|\delta_\tau \mathbb{e}_h^{\phi,1}\right\|_{-1,h}^2$$
$$\le \frac{C}{\tau}\int_{t_0}^{t_1}\|\partial_{ss}\phi(s)-P_h\partial_{ss}\phi(s)\|_{2,h}^2\,ds+\frac{\beta}{16}\left\|\delta_\tau \mathbb{e}_h^{\phi,1}\right\|_{-1,h}^2,$$

with the assumption that $\partial_t\phi(0)=0$. Additionally, the seventh and ninth terms on the right-hand side of (35) can be bounded as follows:

$$\left(\mathbb{e}_R^{\mu,m}, \delta_\tau \mathbb{e}_h^{\phi,m}\right) \le C\left\|\nabla \mathbb{e}_R^{\mu,m}\right\|_{L^2}^2+\frac{\beta}{16}\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2, \tag{47}$$

and

$$2\left(\nabla\phi^m-\nabla\phi^{m-1}, \nabla\delta_\tau \mathbb{e}_h^{\phi,m}\right) = -2\left(\tau\Delta\delta_\tau\phi^m, \delta_\tau \mathbb{e}_h^{\phi,m}\right)$$
$$\le 2\left\|\tau\nabla\Delta\delta_\tau\phi^m\right\|_{L^2}\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}$$
$$\le C\tau\int_{t_{m-1}}^{t_m}\|\partial_s\phi(s)\|_{H^3}^2\,ds+\frac{\beta}{16}\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2, \tag{48}$$

where we have used (41) to obtain (48). For the nonlinear term, we use properties (40) and (41) along with Lemma 6 and Young's, Hölder's, and Poincaré inequalities and the higher-regularities (29) to obtain,

$$-\left(\left(\phi^m\right)^3-\left(\phi_h^m\right)^3, \delta_\tau \mathbb{e}_h^{\phi,m}\right) \le \left\|\nabla\left(\left(\phi^m\right)^3-\left(\phi_h^m\right)^3\right)\right\|_{L^2}\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}$$
$$=\left\|3\left(\phi^m\right)^2\nabla\phi^m-3\left(\phi_h^m\right)^2\nabla\phi_h^m\right\|_{L^2}\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}$$
$$=3\left\|\left(\phi^m+\phi_h^m\right)\nabla\phi^m \mathbb{e}^{\phi,m}+\left(\phi_h^m\right)^2\nabla \mathbb{e}^{\phi,m}\right\|_{L^2}\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}$$
$$\le 3\left(\left\|\phi^m+\phi_h^m\right\|_{L^6}\left\|\nabla\phi^m\right\|_{L^6}\left\|\mathbb{e}^{\phi,m}\right\|_{L^6}+\left\|\phi_h^m\right\|_{L^6}^2\left\|\nabla \mathbb{e}^{\phi,m}\right\|_{L^6}\right)\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}$$
$$\le C\left(\left\|\nabla \mathbb{e}_P^{\phi,m}\right\|_{L^2}+\left\|\nabla \mathbb{e}_h^{\phi,m}\right\|_{L^2}+\left\|\mathbb{e}_P^{\phi,m}\right\|_{2,h}+\left\|\mathbb{e}_h^{\phi,m}\right\|_{2,h}\right)\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}$$
$$\le C\left\|\mathbb{e}_P^{\phi,m}\right\|_{2,h}^2+C\left\|\mathbb{e}_h^{\phi,m}\right\|_{2,h}^2+\frac{\beta}{16}\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2. \tag{49}$$

For the remaining terms, we note that the following discrete product rules hold for any bilinear form and remark that these discrete product rules are key to recovering the predicted error estimates:

$$\begin{aligned}\left(a^{m-1}, \frac{b^m - b^{m-1}}{\tau}\right) &= \frac{1}{\tau}\left[\left(a^m, b^m\right) - \left(a^{m-1}, b^{m-1}\right)\right] - \left(\frac{a^m - a^{m-1}}{\tau}, b^m\right) \\ &= \delta_\tau \left(a^m, b^m\right) - \left(\delta_\tau a^m, b^m\right),\end{aligned}$$

and

$$\begin{aligned}\left(a^{m}, \frac{b^m - b^{m-1}}{\tau}\right) &= \frac{1}{\tau}\left[\left(a^m, b^m\right) - \left(a^{m-1}, b^{m-1}\right)\right] - \left(\frac{a^m - a^{m-1}}{\tau}, b^{m-1}\right) \\ &= \delta_\tau \left(a^m, b^m\right) - \left(\delta_\tau a^m, b^{m-1}\right).\end{aligned}$$

Thus, we have the following bound

$$\begin{aligned}2\left(\nabla \mathbb{e}_P^{\phi,m-1}, \nabla \delta_\tau \mathbb{e}_h^{\phi,m}\right) &= 2\delta_\tau \left(\nabla \mathbb{e}_P^{\phi,m}, \nabla \mathbb{e}_h^{\phi,m}\right) - 2\left(\nabla \delta_\tau \mathbb{e}_P^{\phi,m}, \nabla \mathbb{e}_h^{\phi,m}\right) \\ &\leq 2\delta_\tau \left(\nabla \mathbb{e}_P^{\phi,m}, \nabla \mathbb{e}_h^{\phi,m}\right) + C\left\|\delta_\tau \mathbb{e}_P^{\phi,m}\right\|_{L^2}^2 + C\left\|\mathbb{e}_h^{\phi,m}\right\|_{2,h}^2 \\ &\leq 2\delta_\tau \left(\nabla \mathbb{e}_P^{\phi,m}, \nabla \mathbb{e}_h^{\phi,m}\right) + \frac{C}{\tau}\int_{t_{m-1}}^{t_m} \|\partial_s \phi(s) - P_h \partial_s \phi(s)\|_{2,h}^2 \, ds \\ &\quad + C\left\|\mathbb{e}_h^{\phi,m}\right\|_{2,h}^2. \end{aligned} \tag{50}$$

Additionally invoking Lemma 7 yields,

$$\begin{aligned}&a_h^{IP}\left(\phi^m, \delta_\tau \mathbb{e}_h^{\phi,m} - E_h \delta_\tau \mathbb{e}_h^{\phi,m}\right) + \left(\left(\phi^m\right)^3 + \alpha\phi^m, \delta_\tau \mathbb{e}_h^{\phi,m} - E_h \delta_\tau \mathbb{e}_h^{\phi,m}\right) \\ &\quad - 2\left(\nabla \phi^m, \nabla \delta_\tau \mathbb{e}_h^{\phi,m} - \nabla E_h \delta_\tau \mathbb{e}_h^{\phi,m}\right) - \left(\mu^m, \delta_\tau \mathbb{e}_h^{\phi,m} - E_h \delta_\tau \mathbb{e}_h^{\phi,m}\right) \\ &= \delta_\tau a_h^{IP}\left(\phi^m, \mathbb{e}_h^{\phi,m} - E_h \mathbb{e}_h^{\phi,m}\right) + \delta_\tau\left(\left(\phi^m\right)^3 + \alpha\phi^m, \mathbb{e}_h^{\phi,m} - E_h \mathbb{e}_h^{\phi,m}\right) \\ &\quad - 2\delta_\tau\left(\nabla\phi^m, \nabla\left(\mathbb{e}_h^{\phi,m} - E_h \mathbb{e}_h^{\phi,m}\right)\right) - \delta_\tau\left(\mu^m, \mathbb{e}_h^{\phi,m} - E_h \mathbb{e}_h^{\phi,m}\right) \\ &\quad - a_h^{IP}\left(\delta_\tau\phi^m, \mathbb{e}_h^{\phi,m-1} - E_h \mathbb{e}_h^{\phi,m-1}\right) - \left(\delta_\tau\left(\left(\phi^m\right)^3 + \alpha\phi^m\right), \mathbb{e}_h^{\phi,m-1} - E_h \mathbb{e}_h^{\phi,m-1}\right) \\ &\quad + 2\left(\delta_\tau \nabla\phi^m, \nabla\left(\mathbb{e}_h^{\phi,m-1} - E_h \mathbb{e}_h^{\phi,m-1}\right)\right) + \left(\delta_\tau \mu^m, \mathbb{e}_h^{\phi,m-1} - E_h \mathbb{e}_h^{\phi,m-1}\right) \\ &\leq \delta_\tau a_h^{IP}\left(\phi^m, \mathbb{e}_h^{\phi,m} - E_h \mathbb{e}_h^{\phi,m}\right) + \delta_\tau\left(\left(\phi^m\right)^3 + \alpha\phi^m, \mathbb{e}_h^{\phi,m} - E_h \mathbb{e}_h^{\phi,m}\right) \\ &\quad - 2\delta_\tau\left(\nabla\phi^m, \nabla\left(\mathbb{e}_h^{\phi,m} - E_h \mathbb{e}_h^{\phi,m}\right)\right) - \delta_\tau\left(\mu^m, \mathbb{e}_h^{\phi,m} - E_h \mathbb{e}_h^{\phi,m}\right) \\ &\quad + C\left[\operatorname{Osc}_j(\partial_t \mu(t^*))\right]^2 + C\left\|\mathbb{e}_P^{\phi,m}\right\|_{2,h}^2 + C\left\|\mathbb{e}_h^{\phi,m-1}\right\|_{2,h}^2. \end{aligned} \tag{51}$$

Now applying the polarization property to the appropriate terms on the left-hand side of (35) and combining the resulting inequality with Eqs. (43)–(51), we have

$$\begin{aligned}
&\beta \left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2 + \frac{1}{2}\delta_\tau \left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2 + \frac{1}{2\tau}\left\|\delta_\tau \mathbb{e}_h^{\phi,m} - \delta_\tau \mathbb{e}_h^{\phi,m-1}\right\|_{-1,h}^2 \\
&\quad + \frac{1}{2}\delta_\tau\, a_h^{IP}\left(\mathbb{e}_h^{\phi,m}, \mathbb{e}_h^{\phi,m}\right) + \frac{\tau}{2} a_h^{IP}\left(\delta_\tau \mathbb{e}_h^{\phi,m}, \delta_\tau \mathbb{e}_h^{\phi,m}\right) + \frac{4+\alpha}{2}\delta_\tau \left\|\mathbb{e}_h^{\phi,m}\right\|_{L^2}^2 \\
&\quad + \frac{4+\alpha}{2}\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{L^2}^2 + \tau \left\|\nabla \delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{L^2}^2 \\
&\le \delta_\tau \left(\nabla \mathbb{e}_h^{\phi,m}, \nabla \mathbb{e}_h^{\phi,m}\right) + 2\delta_\tau \left(\nabla \mathbb{e}_P^{\phi,m}, \nabla \mathbb{e}_h^{\phi,m}\right) + \frac{\beta}{2}\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2 + C\left\|\mathbb{e}_h^{\phi,m-1}\right\|_{2,h}^2 \\
&\quad + C\left\|\mathbb{e}_h^{\phi,m}\right\|_{2,h}^2 + C\left\|\nabla \mathbb{e}_R^{\mu,m}\right\|_{L^2}^2 + C\left\|\mathbb{e}_P^{\phi,m}\right\|_{2,h}^2 + C\left[\mathrm{Osc}_j(\partial_t \mu(t^*))\right]^2 \\
&\quad + C\tau \int_{t_{m-1}}^{t_m}\left[\|\partial_s \phi(s)\|_{L^2}^2 + \|\partial_{ss}\phi(s)\|_{L^2}^2\right] ds + C\tau \int_{t_{m-2}}^{t_m}\left[\|\partial_{sss}\phi(s)\|_{L^2}^2\right] ds \\
&\quad + \frac{C}{\tau}\int_{t_{m-2}}^{t_m}\|\partial_{ss}\phi(s) - P_h \partial_{ss}\phi(s)\|_{2,h}^2\, ds + \frac{C}{\tau}\int_{t_{m-1}}^{t_m}\|\partial_s \phi(s) - P_h \partial_s \phi(s)\|_{2,h}^2\, ds \\
&\quad + \delta_\tau a_h^{IP}\left(\phi^m, \mathbb{e}_h^{\phi,m} - E_h \mathbb{e}_h^{\phi,m}\right) + \delta_\tau \left((\phi^m)^3 + \alpha\phi^m, \mathbb{e}_h^{\phi,m} - E_h \mathbb{e}_h^{\phi,m}\right) \\
&\quad - 2\delta_\tau \left(\nabla \phi^m, \nabla\left(\mathbb{e}_h^{\phi,m} - E_h \mathbb{e}_h^{\phi,m}\right)\right) - \delta_\tau \left(\mu^m, \mathbb{e}_h^{\phi,m} - E_h \mathbb{e}_h^{\phi,m}\right),
\end{aligned}$$

with $t_{-1} \equiv t_0$.

Combining like terms, applying $2\tau \sum_{m=1}^{\ell}$, using the fact that $\mathbb{e}_h^{\phi,0} = 0$, invoking Lemma 3, and applying Hölder's inequality, we obtain

$$\begin{aligned}
&a_h^{IP}\left(\mathbb{e}_h^{\phi,\ell}, \mathbb{e}_h^{\phi,\ell}\right) + \left\|\mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2 + (4+\alpha)\left\|\mathbb{e}_h^{\phi,\ell}\right\|_{L^2}^2 + \sum_{m=1}^{\ell}\left\|\delta_\tau \mathbb{e}_h^{\phi,m} - \delta_\tau \mathbb{e}_h^{\phi,m-1}\right\|_{-1,h}^2 \\
&\quad + \tau \sum_{m=1}^{\ell}\left(\beta \left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2 + (4+\alpha)\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{L^2}^2\right) \\
&\quad + \tau^2 \sum_{m=1}^{\ell}\left[a_h^{IP}\left(\delta_\tau \mathbb{e}_h^{\phi,m}, \delta_\tau \mathbb{e}_h^{\phi,m}\right) + 2\left\|\nabla \delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{L^2}^2\right] \\
&\le 2\sqrt{1+\gamma}\left\|\mathbb{e}_h^{\phi,\ell}\right\|_{L^2}\left\|\mathbb{e}_h^{\phi,\ell}\right\|_{2,h} + 4\sqrt{1+\gamma}\left\|\mathbb{e}_P^{\phi,\ell}\right\|_{L^2}\left\|\mathbb{e}_h^{\phi,\ell}\right\|_{2,h} + C\tau \sum_{m=1}^{\ell}\left\|\mathbb{e}_h^{\phi,m}\right\|_{2,h}^2 \\
&\quad + C\tau \sum_{m=1}^{\ell}\left[\left\|\nabla \mathbb{e}_R^{\mu,m}\right\|_{L^2}^2 + \left\|\mathbb{e}_P^{\phi,m}\right\|_{2,h}^2 + \left[\mathrm{Osc}_j(\partial_t \mu(t^*))\right]^2\right] \\
&\quad + C\int_{t_0}^{t_\ell}\|\partial_{ss}\phi(s) - P_h \partial_{ss}\phi(s)\|_{2,h}^2\, ds + C\int_{t_0}^{t_\ell}\|\partial_s \phi(s) - P_h \partial_s \phi(s)\|_{2,h}^2\, ds \\
&\quad + C\tau^2 \int_{t_0}^{t_\ell}\left[\|\partial_s \phi(s)\|_{L^2}^2 + \|\partial_{ss}\phi(s)\|_{L^2}^2 + \|\partial_{sss}\phi(s)\|_{L^2}^2\right] ds \\
&\quad + 2\Big[a_h^{IP}\left(\phi^\ell, \mathbb{e}_h^{\phi,\ell} - E_h \mathbb{e}_h^{\phi,\ell}\right) + \left(\left(\phi^\ell\right)^3 + \alpha\phi^\ell, \mathbb{e}_h^{\phi,\ell} - E_h \mathbb{e}_h^{\phi,\ell}\right) \\
&\quad - 2\left(\nabla \phi^\ell, \nabla\left(\mathbb{e}_h^{\phi,\ell} - E_h \mathbb{e}_h^{\phi,\ell}\right)\right) - \left(\mu^\ell, \mathbb{e}_h^{\phi,\ell} - E_h \mathbb{e}_h^{\phi,\ell}\right)\Big].
\end{aligned}$$

Applying Young's and Hölder's inequalities and Lemma 7 yields,

$$
\begin{aligned}
& a_h^{IP}\left(\mathbb{e}_h^{\phi,\ell}, \mathbb{e}_h^{\phi,\ell}\right) + \left\|\mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2 + (4+\alpha)\left\|\mathbb{e}_h^{\phi,\ell}\right\|_{L^2}^2 + \sum_{m=1}^{\ell}\left\|\delta_\tau \mathbb{e}_h^{\phi,m} - \delta_\tau \mathbb{e}_h^{\phi,m-1}\right\|_{-1,h}^2 \\
& \quad + \tau\sum_{m=1}^{\ell}\left(\beta\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2 + (4+\alpha)\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{L^2}^2\right) \\
& \quad + \tau^2\sum_{m=1}^{\ell}\left[a_h^{IP}\left(\delta_\tau \mathbb{e}_h^{\phi,m}, \delta_\tau \mathbb{e}_h^{\phi,m}\right) + 2\left\|\nabla\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{L^2}^2\right] \\
& \le \frac{C_{coer}}{2}\left\|\mathbb{e}_h^{\phi,\ell}\right\|_{2,h}^2 + \frac{4(1+\gamma)}{C_{coer}}\left\|\mathbb{e}_h^{\phi,\ell}\right\|_{L^2}^2 + C\left\|\mathbb{e}_P^{\phi,\ell}\right\|_{2,h}^2 + C\tau\sum_{m=1}^{\ell}\left\|\mathbb{e}_h^{\phi,m}\right\|_{2,h}^2 \\
& \quad + C\tau\sum_{m=1}^{\ell}\left[\|\nabla \mathbb{e}_R^{\mu,m}\|_{L^2}^2 + \left\|\mathbb{e}_P^{\phi,m}\right\|_{2,h}^2 + \left[\operatorname{Osc}_j(\partial_t\mu(t^*))\right]^2\right] \\
& \quad + C\int_{t_0}^{t_\ell}\|\partial_s\phi(s) - P_h\partial_s\phi(s)\|_{2,h}^2\, ds \\
& \quad + C\tau^2\int_{t_0}^{t_\ell}\left[\|\partial_s\phi(s)\|_{L^2}^2 + \|\partial_{ss}\phi(s)\|_{L^2}^2 + \|\partial_{sss}\phi(s)\|_{L^2}^2\right] ds \\
& \quad + 2\Big[C\left[\operatorname{Osc}_j(\mu^\ell)\right]^2 + C\left\|\mathbb{e}_P^{\phi,\ell}\right\|_{2,h}^2 + \frac{C_{coer}}{4\kappa}\left\|\mathbb{e}_h^{\phi,\ell}\right\|_{2,h}^2\Big],
\end{aligned}
$$

for $t^* \in (t_{m-1}, t_m)$. Invoking Lemma 1 and combining like terms, we have

$$
\begin{aligned}
& \frac{C_{coer}}{2}\left\|\mathbb{e}_h^{\phi,\ell}\right\|_{2,h}^2 + \left\|\mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2 + \left[\alpha + 4 - \frac{4(1+\gamma)}{C_{coer}}\right]\left\|\mathbb{e}_h^{\phi,\ell}\right\|_{L^2}^2 \\
& \quad + C\sum_{m=1}^{\ell}\left\|\delta_\tau \mathbb{e}_h^{\phi,m} - \delta_\tau \mathbb{e}_h^{\phi,m-1}\right\|_{-1,h}^2 + C\,\tau\sum_{m=1}^{\ell}\left(\beta\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2 + (4+\alpha)\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{L^2}^2\right) \\
& \quad + C\tau^2\sum_{m=1}^{\ell}\left[C_{coer}\left\|\delta_\tau \mathbb{e}_h^{\phi,\ell}\right\|_{2,h}^2 + \left\|\nabla\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{L^2}^2\right] \\
& \le C\tau\sum_{m=1}^{\ell}\left\|\mathbb{e}_h^{\phi,m}\right\|_{2,h}^2 + C\left\|\mathbb{e}_P^{\phi,\ell}\right\|_{2,h}^2 + C\left[\operatorname{Osc}_j(\mu^\ell)\right]^2 \\
& \quad + C\tau\sum_{m=1}^{\ell}\left[\|\nabla \mathbb{e}_R^{\mu,m}\|_{L^2}^2 + \left\|\mathbb{e}_P^{\phi,m}\right\|_{2,h}^2 + \left[\operatorname{Osc}_j(\partial_t\mu(t^*))\right]^2\right] \\
& \quad + C\tau^2\int_{t_0}^{t_\ell}\left[\|\partial_s\phi(s)\|_{L^2}^2 + \|\partial_{ss}\phi(s)\|_{L^2}^2 + \|\partial_{sss}\phi(s)\|_{L^2}^2\right] ds \\
& \quad + C\int_{t_0}^{t_\ell}\|\partial_s\phi(s) - P_h\partial_s\phi(s)\|_{2,h}^2\, ds.
\end{aligned}
$$

Requiring $\alpha > \max\left\{\frac{(1+\gamma)}{C_{coer}} - 1, \frac{4(1+\gamma)}{C_{coer}} - 4\right\} > 0$, we have

$$\begin{aligned}
&C_1 \left\|\mathbb{e}_h^{\phi,\ell}\right\|_{2,h}^2 + C\left\|\mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2 + C\left\|\mathbb{e}_h^{\phi,\ell}\right\|_{L^2}^2 + C\sum_{m=1}^{\ell}\left\|\delta_\tau \mathbb{e}_h^{\phi,m} - \delta_\tau \mathbb{e}_h^{\phi,m-1}\right\|_{-1,h}^2 \\
&\quad + C\,\tau\sum_{m=1}^{\ell}\left(\beta\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2 + (4+\alpha)\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{L^2}^2\right) \\
&\quad + C\tau^2\sum_{m=1}^{\ell}\left[C_{coer}\left\|\delta_\tau \mathbb{e}_h^{\phi,\ell}\right\|_{2,h}^2 + (4+\alpha)\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{L^2}^2 + \left\|\nabla\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{L^2}^2\right] \\
&\le C_2\tau\sum_{m=1}^{\ell}\left\|\mathbb{e}_h^{\phi,m}\right\|_{2,h}^2 + C\left\|\mathbb{e}_P^{\phi,\ell}\right\|_{2,h}^2 + C\left[\mathrm{Osc}_j(\mu^\ell)\right]^2 \\
&\quad + C\tau\sum_{m=1}^{\ell}\left[\|\nabla \mathbb{e}_R^{\mu,m}\|_{L^2}^2 + \left\|\mathbb{e}_P^{\phi,m}\right\|_{2,h}^2 + \left[\mathrm{Osc}_j(\partial_t\mu(t^*))\right]^2\right] \\
&\quad + C\tau^2\int_{t_0}^{t_\ell}\left[\|\partial_s\phi(s)\|_{L^2}^2 + \|\partial_{ss}\phi(s)\|_{L^2}^2 + \|\partial_{sss}\phi(s)\|_{L^2}^2\right]ds \\
&\quad + C\int_{t_0}^{t_\ell}\|\partial_s\phi(s) - P_h\partial_s\phi(s)\|_{2,h}^2\,ds \\
&\le C_2\tau\sum_{m=1}^{\ell}\left\|\mathbb{e}_h^{\phi,m}\right\|_{2,h}^2 + C\left\|\mathbb{e}_P^{\phi,\ell}\right\|_{2,h}^2 + C\left[\mathrm{Osc}_j(\mu^\ell)\right]^2 \\
&\quad + C\tau\sum_{m=1}^{\ell}\left[Ch^2|\mu|_{H^2(\Omega)}^2 + \left\|\mathbb{e}_P^{\phi,m}\right\|_{2,h}^2 + \left[\mathrm{Osc}_j(\partial_t\mu(t^*))\right]^2\right] \\
&\quad + C\tau^2\int_{t_0}^{t_\ell}\left[\|\partial_s\phi(s)\|_{L^2}^2 + \|\partial_{ss}\phi(s)\|_{L^2}^2 + \|\partial_{sss}\phi(s)\|_{L^2}^2\right]ds \\
&\quad + C\int_{t_0}^{t_\ell}\|\partial_s\phi(s) - P_h\partial_s\phi(s)\|_{2,h}^2\,ds,
\end{aligned}$$

where we have used well-known properties of the Ritz projection operator (32) in the last step. Combining like terms and considering the higher regularities (29) and the fact that $\mathrm{Osc}_j(f) \le Ch^2$ for some function $f \in L^2(\Omega)$, we have

$$\begin{aligned}
&\left\|\mathbb{e}_h^{\phi,\ell}\right\|_{2,h}^2 + C\left\|\mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2 + C\left\|\mathbb{e}_h^{\phi,\ell}\right\|_{L^2}^2 + C\sum_{m=1}^{\ell}\left\|\delta_\tau \mathbb{e}_h^{\phi,m} - \delta_\tau \mathbb{e}_h^{\phi,m-1}\right\|_{-1,h}^2 \\
&\quad + C\,\tau\sum_{m=1}^{\ell}\left(\beta\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{-1,h}^2 + (4+\alpha)\left\|\delta_\tau \mathbb{e}_h^{\phi,m}\right\|_{L^2}^2\right)
\end{aligned}$$

Table 1 Errors and convergence rates

h	$\|error_\phi\|_{2,h}$	Rate
32/8	0.19323	N/A
32/16	0.04071	2.37325
32/32	0.02017	1.00917
32/64	0.00741	1.36099
32/128	0.00269	1.37732

Parameters and initial conditions are given in the text

$$+ C\tau^2 \sum_{m=1}^{\ell} \left[C_{coer} \left\| \delta_\tau \mathbb{e}_h^{\phi,\ell} \right\|_{2,h}^2 + (4+\alpha) \left\| \delta_\tau \mathbb{e}_h^{\phi,m} \right\|_{L^2}^2 + \left\| \nabla \delta_\tau \mathbb{e}_h^{\phi,m} \right\|_{L^2}^2 \right]$$
$$\leq \frac{C_2\tau}{C_1 - C_2\tau} \sum_{m=1}^{\ell-1} \left\| \mathbb{e}_h^{\phi,m} \right\|_{2,h}^2 + C \left\| \mathbb{e}_P^{\phi,\ell} \right\|_{2,h}^2 + C\tau \sum_{m=1}^{\ell} \left\| \mathbb{e}_P^{\phi,m} \right\|_{2,h}^2$$
$$+ C \int_{t_0}^{t_\ell} \|\partial_s \phi(s) - P_h \partial_s \phi(s)\|_{2,h}^2 \, ds + C(T+1)h^2 + C\tau^2.$$

Allowing for $0 < \tau < \tau_0$ such that $\tau_0 := \frac{C_1}{C_2}$, noting the higher regularities (29), and using the Ritz projection properties [15] we have

$$\left\| \mathbb{e}_h^{\phi,\ell} \right\|_{2,h}^2 + C \left\| \mathbb{e}_h^{\phi,m} \right\|_{-1,h}^2 + C \left\| \mathbb{e}_h^{\phi,\ell} \right\|_{L^2}^2 + C \sum_{m=1}^{\ell} \left\| \delta_\tau \mathbb{e}_h^{\phi,m} - \delta_\tau \mathbb{e}_h^{\phi,m-1} \right\|_{-1,h}^2$$
$$+ C\,\tau \sum_{m=1}^{\ell} \left(\beta \left\| \delta_\tau \mathbb{e}_h^{\phi,m} \right\|_{-1,h}^2 + (4+\alpha) \left\| \delta_\tau \mathbb{e}_h^{\phi,m} \right\|_{L^2}^2 \right)$$
$$+ C\tau^2 \sum_{m=1}^{\ell} \left[C_{coer} \left\| \delta_\tau \mathbb{e}_h^{\phi,\ell} \right\|_{2,h}^2 + (4+\alpha) \left\| \delta_\tau \mathbb{e}_h^{\phi,m} \right\|_{L^2}^2 + \left\| \nabla \delta_\tau \mathbb{e}_h^{\phi,m} \right\|_{L^2}^2 \right]$$
$$\leq C_3\tau \sum_{m=1}^{\ell-1} \left\| \mathbb{e}_h^{\phi,m} \right\|_{2,h}^2 + C((T+1)h^2 + \tau^2),$$

where none of the constants above depend on the mesh size h or the time step size τ. Applying a discrete Grönwall's concludes the proof.

Remark 5 Again following [3], we note that C_{coer} can be chosen to be close to 1 as long as the penalty parameter σ is large enough. In this case, γ could also be chosen close to 0 and (39) will hold as long as $\alpha > 0$.

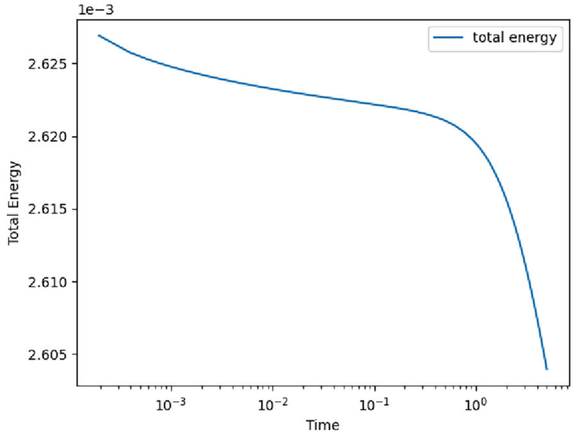

Fig. 2 The time evolution of the scaled total energy $F/32^2$. The mesh size is $h = 32/256$ and the time step size is $\tau = 0.05h$. All other parameters are defined in the text

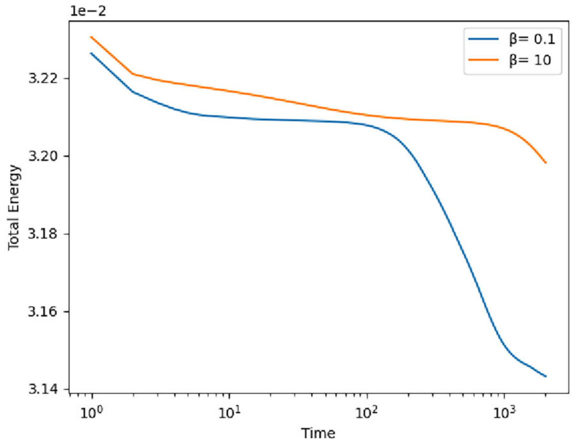

Fig. 3 The time evolution of the scaled total energy $F/201^2$ with $\beta = 0.1$ and $\beta = 10$. All other parameters are defined in the text

5 Numerical Experiments

In this section, we present two numerical experiments demonstrating the effectiveness of our method. Both numerical experiments are completed using the Firedrake project [20]. Furthermore, in order to avoid a two-step time-stepping scheme, we introduce an auxiliary variable $\psi_h^m := \delta_\tau \phi_h^m$ as in [1, 34] and solve the following problem: given $\phi_h^{m-1}, \psi_h^{m-1} \in Z_h \times Z_h$, find $\phi_h^m, \mu_h^m \in Z_h \times Z_h$ such that for all $\nu_h, z_h \in Z_h$

$$\frac{1+\beta\tau}{\tau^2}\left(\phi_h^m - \phi_h^{m-1}, \nu_h\right) - \frac{1}{\tau}\left(\psi_h^{m-1}, \nu_h\right) + \left(\nabla\mu_h^m, \nabla\nu_h\right) = 0, \quad (52a)$$

$$a_h^{IP}\left(\phi_h^m, z_h\right) + \left(\left(\phi_h^m\right)^3 + \alpha\,\phi_h^m, z_h\right) - 2\left(\nabla\phi_h^{m-1}, \nabla z_h\right) - \left(\mu_h^m, z_h\right) = 0, \quad (52b)$$

and then update $\psi_h^m = \dfrac{\phi_h^m - \phi_h^{m-1}}{\tau}$.

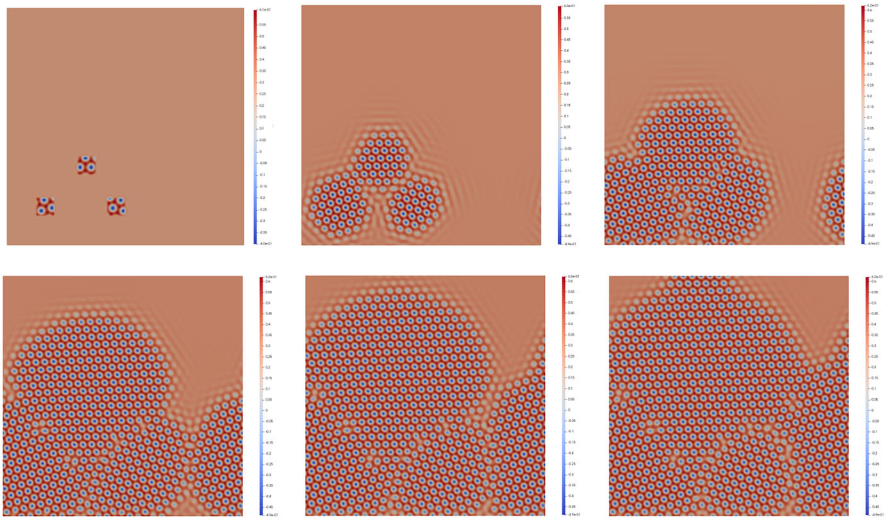

Fig. 4 Snapshots of grain growth at times $T = 0, 250, 500, 1000, 1500, 2000$ with $\beta = 0.1$. All other parameters are defined in the text

In our first experiment, we show that our method converges with first order accuracy with regard to both time and space in Table 1. We furthermore show that the discrete energy (24) dissipates over time in Fig. 2. Following [1], we set the initial conditions to be

$$\phi(x, y) = 0.07 - 0.02 \cos\left(\frac{2\pi(x-12)}{32}\right) \sin\left(\frac{2\pi(y-1)}{32}\right) + 0.02 \cos^2\left(\frac{\pi(x+10)}{32}\right) \cos^2\left(\frac{\pi(y+3)}{32}\right) - 0.01 \sin^2\left(\frac{4\pi x}{32}\right) \sin^2\left(\frac{4\pi(y-6)}{32}\right)$$

and solve on the domain $\Omega = (0, 32) \times (0, 32)$ to a final stopping time of $T = 2$. We solve using the mesh sizes shown in the table below and scale the time step size with the mesh size via $\tau = 0.05h$. We set $\beta = 0.9$, $\alpha = 0.975$ and the penalty parameter $\sigma = 20$. We point out that Neumann boundary conditions are implemented. To show first order convergence in the energy norm, we assign the solution from a mesh size of $h = 32/256$ with $\tau = 0.05h$ and $T = 2$ as the 'exact' solution, ϕ_{exact}. We then define $error_\phi := \phi_h - \phi_{exact}$, where ϕ_h indicates the solution on the mesh size h with $\tau = 0.05h$ and $T = 2$. Table 1 shows the errors and rates of convergence given the parameters noted in the text above.

In the second experiment, we demonstrate the effectiveness of our method in capturing the process of grain growth. For the initial conditions, we define three crystallites with different orientations as in [21]. We then solve on the domain $\Omega = (0, 201) \times (0, 201)$ to a final stopping time of $T = 2000$ and enforce peri-

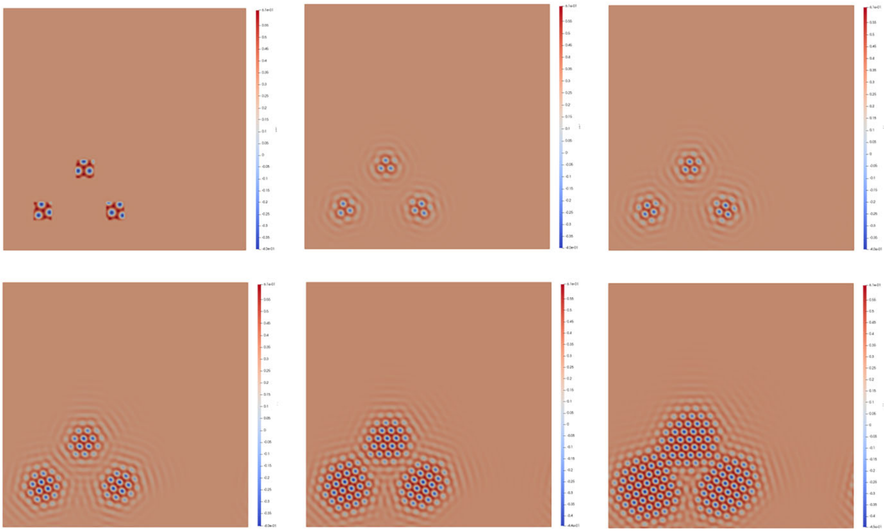

Fig. 5 Snapshots of grain growth at times $T = 0, 250, 500, 1000, 1500, 2000$ with $\beta = 10$. All other parameters are defined in the text

odic boundary conditions. The mesh size is taken to be $h = 201/512$, the time step size is taken to be $\tau = 1$, the parameter α is set to 0.75, and the penalty parameter σ is set to 10. We run the experiment twice under two different values of β; first with $\beta = 0.1$ and then with $\beta = 10$. As demonstrated in Baskaran et al. [1], we expect the grain growth to develop more quickly with $\beta = 0.1$ than with $\beta = 10$ due to the dominance of the term involving the second derivative in time in the MPFC model (1). Figures 4 and 5 demonstrate that the C^0-IP method realizes this expectation. We also observe well-defined crystal–liquid interfaces as expected. Similarly, a difference in the energy dissipation is also observed in Fig. 3.

The authors would like to mention that the second author was an undergraduate student during the time in which research on this project was completed and contributed by helping to code and implement the numerical experiments. He has since moved to a different university as a graduate student.

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Declarations

Conflict of interest On behalf of all authors, the corresponding author states that there is no conflict of interest.

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