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Convergence analysis for second-order accurate schemes for the periodic nonlocal Allen-Cahn and Cahn-Hilliard equations

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In this paper, we provide a detailed convergence analysis for fully discrete second-order (in both time and space) numerical schemes for nonlocal Allen-Cahn and nonlocal Cahn-Hilliard equations. The unconditional unique solvability and energy stability ensures ℓ^4 stability. The convergence analysis for the nonlocal Allen-Cahn equation follows the standard procedure of consistency and stability estimate for the numerical error function. For the nonlocal Cahn-Hilliard equation, because of the complicated form of the nonlinear term, a careful expansion of its discrete gradient is undertaken, and an H^{-1} inner-product estimate of this nonlinear numerical error is derived to establish convergence. In addition, an a priori $W^{1,\infty}$ bound of the numerical solution at the discrete level is needed in the error estimate. Such a bound can be obtained by performing a higher order consistency analysis by using asymptotic expansions for the numerical solution. Following the technique originally proposed by Strang (eg, 1964), instead of the standard comparison between the exact and numerical solutions, an error estimate between the numerical solution and the constructed approximate solution yields an $O(s^3 + h^4)$ convergence in $\ell^\infty(0, T; \ell^2)$ norm, in which s and h denote the time step and spatial mesh sizes, respectively. This in turn leads to the necessary bound under a standard constraint $s \le Ch$. Here, we also prove convergence of the scheme in the maximum norm under the same constraint.

KEYWORDS

convergence analysis, energy stability, higher order asymptotic expansion, nonlocal Allen-Cahn equation, nonlocal Cahn-Hilliard equation, second-order numerical scheme

1 | INTRODUCTION

In this paper, our primary goal is to develop a detailed convergence analysis of fully discrete second-order (in both time and space) numerical schemes for nonlocal Allen-Cahn (nAC) and nonlocal Cahn-Hilliard (nCH) equations, which are integro-partial-differential equations (IPDEs) defined as follows:

$$\partial_t \phi = -M(\phi) w \quad \text{(nAC)}, \tag{1.1}$$

and

$$\partial_t \phi = \nabla \cdot (M(\phi) \nabla w) \quad \text{(nCH)}, \tag{1.2}$$

where

$$w := \delta_\phi E = \phi^3 + \gamma_c \phi - \gamma_e \phi + (\mathrm{J} * 1)\phi - \mathrm{J} * \phi \tag{1.3}$$

and $M(\phi) \geqslant 0$ is the mobility. These equations are defined in $(0, T] \times \Omega$, with the initial condition

$$\phi(0, x) = \phi_0(x), \tag{1.4}$$

where Ω is a rectangular domain in $\mathbb{R}^n$. The solution $\phi(x, t)$ is Ω-periodic in space. The convolution kernel J is also Ω-periodic and even. By $\mathsf{J} * \phi$, we mean the circular, or periodic, convolution defined as

$$(\mathsf{J} * \phi)(\mathbf{x}) := \int_\Omega \mathsf{J}(\mathbf{y})\, \phi(\mathbf{x} - \mathbf{y})\, d\mathbf{y} = \int_\Omega \mathsf{J}(\mathbf{x} - \mathbf{y})\, \phi(\mathbf{y})\, d\mathbf{y}, \tag{1.5}$$

in which $\gamma_c \geqslant 0$ and $\gamma_e \geqslant 0$ are system parameters. For the convenience of analysis, we use the form $\gamma_c - \gamma_e$ instead of merging them together. The term w defined in (1.3) is the chemical potential (variational derivative) relative to the energy

$$E(\phi) = \int_\Omega \left\{ \frac{1}{4}\phi^4 + \frac{\gamma_c - \gamma_e}{2}\phi^2 + \frac{1}{4}\int_\Omega \mathsf{J}(\mathbf{x} - \mathbf{y})(\phi(\mathbf{x}) - \phi(\mathbf{y}))^2 d\mathbf{y} \right\} d\mathbf{x}. \tag{1.6}$$

Equations 1.1 and 1.2 are L^2 (nAC) and H^{-1} (nCH) flows of $E(\phi)$ and their periodic solutions dissipate E at the rate $d_t E(\phi) = -\sqrt{M}\|w\|_{L^2}^2$, $d_t E(\phi) = -\sqrt{M}\,\|\nabla w\|_{L^2}^2$, respectively.

Equations 1.1 and 1.2 are members of a more general family of IPDE models:

$$\partial_t \phi = -M(\phi) w_{general} \quad \text{(nAC)}, \tag{1.7}$$

and

$$\partial_t \phi = \nabla \cdot (M(\phi) \nabla w_{general}) \quad \text{(nCH)}, \tag{1.8}$$

where

$$w_{general} := \delta_\phi E = F'(\phi) + (\mathsf{J} * 1)\phi - \mathsf{J} * \phi. \tag{1.9}$$

The energy $E_{general}(\phi)$ associated with this model is defined as

$$E_{general}(\phi) = \int_\Omega \left\{ F(\phi) + \frac{1}{4}\int_\Omega \mathsf{J}(\mathbf{x} - \mathbf{y})(\phi(\mathbf{x}) - \phi(\mathbf{y}))^2 d\mathbf{y} \right\} d\mathbf{x}, \tag{1.10}$$

where $F(\phi)$ is the local energy density and it is usually nonlinear. The classical Allen-Cahn (AC) and Cahn-Hilliard (CH) equations are the approximation to this type of IPDE models, whose free energy[1-3] is

$$E_{\text{local}}(\phi) = \int_\Omega \left(G(\phi) + \frac{\epsilon^2}{2}|\nabla \phi|^2 \right) d\mathbf{x}, \tag{1.11}$$

and the corresponding dynamical equations are

$$\partial_t \phi = -\left(M(\phi)\delta_\phi E_{\text{local}}\right) = -\left(M(\phi)\left(G'(\phi) - \epsilon^2 \Delta \phi\right)\right) \quad \text{(AC)}, \tag{1.12}$$

and

$$\partial_t \phi = \nabla \cdot \left(M(\phi)\nabla \delta_\phi E_{\text{local}}\right) = \nabla \cdot \left(M(\phi)\nabla\left(G'(\phi) - \epsilon^2 \Delta \phi\right)\right) \quad \text{(CH)}. \tag{1.13}$$

The approximation is established as follows.[4-8] By Taylor's expansion, $(\mathsf{J} * \phi) \approx \mathsf{J}_0 \phi + \frac{1}{2}\mathsf{J}_2 \Delta \phi$. Here, $\mathsf{J}_0 = \int_\Omega \mathsf{J}(\mathbf{x}) d\mathbf{x}$ and $\mathsf{J}_2 = \int_\Omega \mathsf{J}(\mathbf{x})|\mathbf{x}|^2\, d\mathbf{x}$ (J_2 is the second moment of J). Under the assumption of periodic boundary conditions, we have the following approximation:

$$\frac{1}{2}(\phi, \mathsf{J} * \phi)_{L^2} \approx \frac{1}{2}\left(\phi, \mathsf{J}_0 \phi + \frac{1}{2} J_2 \Delta \phi\right)_{L^2} = \frac{\mathsf{J}_0}{2}\left(\phi^2, \mathbf{1}\right)_{L^2} + \frac{\mathsf{J}_2}{4}\int_\Omega |\nabla \phi|^2 d\mathbf{x}. \tag{1.14}$$

On the other hand, the energy E_{general} is equivalent to

$$E_{\text{general}}(\phi) = (F(\phi), 1)_{L^2} - \frac{1}{2}(\phi, \mathsf{J} * \phi)_{L^2}. \tag{1.15}$$

Denote $G(\phi) = F(\phi) - \frac{\mathsf{J}_0}{2}\phi^2$ and $\epsilon^2 = \frac{\mathsf{J}_2}{2}$, we can obtain $E_{\text{local}} \approx E_{\text{general}}$.

General nCH and nAC equations such as Equations 1.7 and 1.8 have been widely used in many fields ranging from physics and material science to biology, finance, and image processing. In material science, Equation 1.8 and other closely related models arise as mesoscopic models of interacting particle systems.[7,9,10] Equation 1.7 is also used to model phase transition.[11] For instance, in dynamic density functional theory model,[4,9] the interaction kernel $\mathsf{J} = c^{(2)}(x, y|\phi_{ref})$ is the 2-particle direct correlation function, ϕ represents the mesoscopic particle density, and ϕ_{ref} is the average density. Another example is the

structural phase field crystal model. It is developed to model the evolution of materials in diffusive scale, while maintaining atomic resolution.[12] The structural phase field crystal model and its extensions have been used in many researches for material science since.[13-15] Readers are referred to previous studies[6,8,16-20] for further details. In biology, Equation 1.8 has been used to model the tissue growth that covers both bulk and cellular levels. In these models, J has been used to model interactions among cells and extracellular matrix.[21-24] Equation 1.7 has also been used in mathematical models of finance. In this case, J arises from an expectation taken with respect to a particular measure that is used in the model for option pricing.[25] In the modeling for image segmentation with nCH equation, J is interpreted as the attracting force.[26,27] Readers are referred to previous works[27-35] for theoretical studies of general nCH equations and another studies[5,11,36] for general nAC equations. The nCH equation has also been extended to model hydrodynamics with the coupling of Navier-Stokes–type dynamics.[37-39]

There are a few works dedicated to numerical simulation of, or numerical methods for, equations like (1.1) and (1.2). Anitescu et al[40] considered an implicit-explicit time stepping framework for a nonlocal system modeling turbulence, where, as here, the nonlocal term is treated explicitly. References Du et al and Zhou et al[41,42] address finite element approximations (in space) of nonlocal peridynamic equations with various boundary conditions. In Bates et al,[43] a finite-difference method for Equation 1.1 with nonperiodic boundary conditions is applied and analyzed. Reference Hartley et al[44] uses a spectral-Galerkin method to solve a nAC-type problem, like Equation 1.1, but with a stochastic noise term and equation modeling heat flow. The spectral method is also studied for nAC equation.[45] For other references for equations like (1.2), see previous works.[7,26,46,47] A first-order convex splitting for Equation 1.2 scheme was introduced and analyzed in Guan et al.[48] The scheme is also extended to nonlocal hydrodynamics.[49] A second-order convex splitting scheme for the general system Equation 1.8 was introduced in Guan et al[50]; its unconditional energy stability and unique solvability were presented.

Here, we present a detailed convergence analysis of fully discrete second-order convex splitting schemes using the specific forms of Equations 1.1 and 1.2. We prove convergence in both the ℓ^2 and ℓ^∞ spatial norms. We note that this convergence analysis is much more challenging than that of the first-order scheme, primarily because of its complicated form for the nonlinear term and lack of higher order diffusion term. The present work focuses on the 2D case but can be straightforwardly extended to 3D. Although the result cannot be easily extended to more general nonlinear local densities F, our results are still useful because polynomial local density functions are widely used.

The outline of the paper is given as follows. In Section 2, we define the fully discrete second-order scheme and give some of its basic properties, including energy stability and unique solvability. The second-order convergence analysis for the nAC equation is presented in Section 3. In Section 4, we provide a higher order consistency analysis for the nCH equation, up to order $O(s^3 + h^4)$. In Section 5, we give the details of the convergence analyses for the nCH equation, in both $\ell^\infty(0,T;\ell^2)$ and $\ell^\infty(0,T;\ell^\infty)$ norms. Finally, some numerical results are presented in Section 6, which confirm convergence of the schemes. Some concluding remarks are given in Section 7.

2 | THE SECOND-ORDER CONVEX SPLITTING SCHEMES

2.1 | The discrete periodic convolution and useful inequalities

Denote Ω to be a rectangular domain in $\mathbb{R}^2$. Assume convolution kernel J satisfies

A1. $\mathsf{J} = \mathsf{J}_c - \mathsf{J}_e$, where J_c, J_e are smooth, Ω-periodic, and nonnegative.
A2. J_c and J_e are even, ie, $\mathsf{J}_\alpha(x_1,x_2) = \mathsf{J}_\alpha(-x_1,-x_2)$, for all $x_1, x_2 \in \mathbb{R}$, $\alpha = c, e$.

A1 is used in the convexity analysis for the energy, and A2 is the result of periodic convolution. The energy (1.6) is equivalent to

$$E(\phi) = \frac{1}{4}\|\phi\|_{L^4}^4 + \frac{\gamma_c - \gamma_e + \mathsf{J} * 1}{2}\|\phi\|_{L^2}^2 - \frac{1}{2}(\phi, \mathsf{J} * \phi)_{L^2}. \tag{2.1}$$

Equations 1.1 and 1.2 can also be rewritten as

$$\partial_t \phi = -M(\phi)(a(\phi)\phi - \mathsf{J} * \phi), \quad \text{(nAC)}, \tag{2.2}$$

$$\partial_t \phi = \nabla \cdot (a(\phi)M(\phi)\nabla\phi) - \nabla \cdot (M(\phi)\nabla \mathsf{J} * \phi), \quad \text{(nCH)}, \tag{2.3}$$

where

$$a(\phi) = 3\phi^2 + \gamma_c - \gamma_e + \mathsf{J} * 1. \tag{2.4}$$

We refer to $a(\phi)$ as the diffusive mobility or just the diffusivity. To make Equation 1.2 positive diffusive (and nondegenerate), we require[30]

$$\gamma_c - \gamma_e + \mathsf{J} * 1 =: \gamma_0 > 0, \tag{2.5}$$

in which $a(\phi) > 0$. We will assume that (2.5) holds in the sequel. In this paper, we focus on Equations 1.1 and 1.2, which are a special case of general nAC and nCH equations. They can be obtained by denoting local energy density F as

$$F(\phi) = \frac{1}{4}\phi^4 + \frac{\tilde{\gamma}_c - \tilde{\gamma}_e}{2}\phi^2, \tag{2.6}$$

where $\tilde{\gamma}_c,\ \tilde{\gamma}_e \geqslant 0$ are constants. By rewriting the nonlocal part of E_{general} as

$$-\frac{1}{2}\int_\Omega\int_\Omega \mathsf{J}(\mathbf{x}-\mathbf{y})\phi(\mathbf{x})\phi(\mathbf{y})d\mathbf{y}d\mathbf{x} = \frac{1}{4}\int_\Omega\int_\Omega \mathsf{J}(\mathbf{x}-\mathbf{y})(\phi(\mathbf{x})-\phi(\mathbf{y}))^2 d\mathbf{y}d\mathbf{x} - \int_\Omega \frac{\mathsf{J}*1}{2}\phi^2(\mathbf{x})d\mathbf{y}, \tag{2.7}$$

and

$$\tilde{\gamma}_c - \tilde{\gamma}_e = \gamma_c - \gamma_e + \mathsf{J} * 1, \tag{2.8}$$

we can obtain energy (1.6). This local density is the approximation to a regular solution model with free energy

$$F(\phi) := \theta[\phi\log(\phi) + (1-\phi)\log(1-\phi)] - 2\theta_c\phi(1-\phi), \tag{2.9}$$

where θ and θ_c represent the absolute and critical temperatures, respectively.[12,51-53] System parameters $\gamma_c - \gamma_e$ are used to adjust the approximation for different reference states of ϕ.

We need 2 spaces: $\mathcal{C}_{m\times n}$ is the space of cell-centered grid (or lattice) functions, and $\mathcal{V}_{m\times n}$ is the space of vertex-centered grid functions. The precise definitions can be found in Appendix A. The spaces and the following notations have straightforward extensions to 3 dimensions. Suppose $\phi \in \mathcal{C}_{m\times n}$ is periodic and $f \in \mathcal{V}_{m\times n}$ is periodic. The 2D grid inner-products $(\cdot\|\cdot)$, $[\cdot\|\cdot]_{\text{ew}}$, $[\cdot\|\cdot]_{\text{ns}}$ are defined in Appendix A. The discrete convolution operator $\left[f\star\phi\right] : \mathcal{V}_{m\times n}\times\mathcal{C}_{m\times n}\to\mathcal{C}_{m\times n}$ is defined component-wise as

$$\left[f\star\phi\right]_{i,j} := h^2\sum_{k=1}^{m}\sum_{l=1}^{n} f_{k+\frac{1}{2},l+\frac{1}{2}}\phi_{i-k,j-l}. \tag{2.10}$$

Note very carefully that the order is important in the definition of the discrete convolution $[\cdot\ \star\ \cdot]$. The next result follows from the definition of the discrete convolution and simple estimates. The proof is omitted.

Lemma 2.1. *If $\phi,\psi\in\mathcal{C}_{m\times n}$ are periodic and $f\in\mathcal{V}_{m\times n}$ is periodic and even, ie, $f_{i+\frac{1}{2},j+\frac{1}{2}} = f_{-i+\frac{1}{2},-j+\frac{1}{2}}$, for all $i,j\in\mathbb{Z}$, then*

$$\left(\phi\|\left[f\star\psi\right]\right) = \left(\psi\|\left[f\star\phi\right]\right). \tag{2.11}$$

If, in addition, f is nonnegative, then

$$\left|\left(\phi\|\left[f\star\psi\right]\right)\right| \leq \left[f\star\mathbf{1}\right]\left(\frac{\alpha}{2}(\phi\|\phi) + \frac{1}{2\alpha}(\psi\|\psi)\right), \quad \forall\alpha>0. \tag{2.12}$$

The following lemma is cited from Guan et al[48]; the detailed proof can be found there.

Lemma 2.2. *Suppose $\phi\in\mathcal{C}_{m\times n}$ is periodic. Assume that $\mathsf{f}\in C^\infty_{per}(\Omega)$ is even and define its grid restriction via $f_{i+\frac{1}{2},j+\frac{1}{2}} := \mathsf{f}\left(p_{i+\frac{1}{2}}, p_{j+\frac{1}{2}}\right)$, so that $f\in\mathcal{V}_{m\times n}$. Then for any $\alpha>0$, we have*

$$-2h^2\left(\left[f\star\psi\right]\|\Delta_h\phi\right) \leq \frac{C_2}{\alpha}\|\psi\|_2^2 + \alpha\|\nabla_h\phi\|_2^2, \tag{2.13}$$

where C_2 is a positive constant that depends on f but is independent of h.

2.2 | Semi-discrete convex splitting schemes

The second-order (in time) convex splitting scheme for the nAC equation 1.1 and nCH equation 1.2 has been proposed in a recent article,[50] which was proven to be unconditionally solvable and unconditionally energy stable. These schemes follow the convex properties of the energy[48]:

Lemma 2.3. *There exists a nonnegative constant C such that $E(\phi) + C \geqslant 0$ for all $\phi \in L^4_{per}(\Omega)$. More specifically,*

$$\frac{1}{8}\|\phi\|_{L^4}^4 \leq E(\phi) + \frac{(\gamma_c - \gamma_e - 2(J_e * 1))^2}{2}|\Omega|, \tag{2.14}$$

$$\frac{1}{2}\|\phi\|_{L^2}^2 \leq E(\phi) + \frac{(\gamma - \gamma_e - 2(J_e * 1) - 1)^2}{4}|\Omega|. \tag{2.15}$$

If $\gamma_e = 0$, then $E(\phi) \geqslant 0$ for all $\phi \in L^4_{per}(\Omega)$. Furthermore, the energy (2.1) can be written as the difference of convex functionals, ie, $E = E_c - E_e$, where

$$E_c(\phi) = \frac{1}{4}\|\phi\|_{L^4}^4 + \frac{\gamma_c + 2(J_c * 1)}{2}\|\phi\|_{L^2}^2, \tag{2.16}$$

$$E_e(\phi) = \frac{\gamma_e + J_c * 1 + J_e * 1}{2}\|\phi\|_{L^2}^2 + \frac{1}{2}(\phi, J * \phi)_{L^2}. \tag{2.17}$$

Lemma 2.3 shows the estimate of ϕ in $\mathscr{C}^2$ and $\mathscr{C}^4$, as well as a splitting that separates the energy into convex and concave parts. The decomposition above is not unique, but Equations 2.16 and 2.17 will allow us to separate the nonlocal and nonlinear terms, treating the nonlinearity implicitly and the nonlocal term explicitly, without sacrificing numerical stability.

To motivate the fully discrete scheme that will follow later, we here present semi-discrete version and briefly describe its properties. For the sake of simplicity, we denote the mobility $M(\phi)$ to be constant for Equation 1.1 and $M(\phi) \equiv 1$ for Equation 1.2. For the nonconstant mobility case, the second-order algorithm is proposed in Guan et al[50]; the unique solvability and unconditional energy stability are standard, and the convergence proof can be achieved with similar idea, while with many more technical details.

A second-order (in time) convex splitting scheme for the nAC equation 1.1 and nCH equation 1.2 can be constructed as follows: Given $\phi^k \in C^\infty_{\text{per}}(\Omega)$, find $\phi^{k+1},\ w^{k+1} \in C^\infty_{\text{per}}(\Omega)$ such that

$$\phi^{k+1} - \phi^k = -Msw^{k+1/2}, \quad \text{(nAC equation)}, \tag{2.18}$$

$$\phi^{k+1} - \phi^k = s\Delta w^{k+1/2}, \quad \text{(nCH equation)}, \tag{2.19}$$

$$w^{k+1/2} = \eta\left(\phi^k, \phi^{k+1}\right) + (2(J_c * 1) + \gamma_c)\phi^{k+1/2} - (J_c * 1 + J_e * 1 + \gamma_e)\hat{\phi}^{k+1/2} - J * \hat{\phi}^{k+1/2}, \tag{2.20}$$

$$\eta\left(\phi^k, \phi^{k+1}\right) = \frac{1}{4}\left((\phi^k)^2 + (\phi^{k+1})^2\right)\left(\phi^k + \phi^{k+1}\right), \tag{2.21}$$

$$\phi^{k+1/2} = \frac{1}{2}\left(\phi^k + \phi^{k+1}\right), \quad \hat{\phi}^{k+1/2} = \frac{3}{2}\phi^k - \frac{1}{2}\phi^{k-1}, \tag{2.22}$$

where $s > 0$ is the time step size. This scheme respects the convex splitting nature of the energy E given in (2.16) and (2.17): The contribution to the chemical potential corresponding to the convex energy, E_c, is treated implicitly, and the part corresponding to the concave part, E_e, is treated explicitly. Eyre[54] is often credited with proposing the convex splitting methodology for the Cahn-Hilliard and Allen-Cahn equations. The idea is, however, quite general and can be applied to any gradient flow of an energy that splits into convex and concave parts. See, for example, previous studies.[55-58] Moreover, the treatment of the nonlinear term, the convex and concave diffusion terms, given by (2.21) and (2.22), respectively, follows the methodology in an earlier work[59] to derive a second-order accurate convex splitting scheme for the phase field crystal model. Other related works can also be found in Baskaran et al[60] and Shen et al.[61]

We have the following a priori energy law for the solutions of the second-order scheme (2.19) to (2.22). The statement for the fully discrete version appears later in Section 2.4. Their proof can be found in a recent article.[50]

Theorem 2.4. *Suppose the energy $E(\phi)$ is defined in Equation 2.1. For any $s > 0$, the second-order convex splitting scheme, (2.18) or (2.19), with (2.20) to (2.22), has a unique solution $\phi^{k+1},\ w^{k+1/2} \in C^\infty_{per}(\Omega)$. Moreover, by denoting a pseudo energy*

$$\begin{aligned}\mathcal{E}\left(\phi^k, \phi^{k+1}\right) = E\left(\phi^{k+1}\right) + \frac{((J_c * 1) + J_e * 1 + \gamma_c + \gamma_e)}{4}\left\|\phi^{k+1} - \phi^k\right\|_{L^2}^2 \\ + \frac{1}{4}\left(J * \left(\phi^{k+1} - \phi^k\right), \phi^{k+1} - \phi^k\right)_{L^2},\end{aligned} \tag{2.23}$$

we have $\left(\phi^{k+1}-\phi^{k},1\right)=0$ *for any* $k\geqslant 1$ *and*

$$\mathcal{E}\left(\phi^{k},\phi^{k+1}\right)+Ms\left\|w^{k+1/2}\right\|_{L^2}^2\leq\mathcal{E}\left(\phi^{k-1},\phi^{k}\right),\quad \textit{(nAC equation)}, \tag{2.24}$$

$$\mathcal{E}\left(\phi^{k},\phi^{k+1}\right)+s\left\|\nabla w^{k+1/2}\right\|_{L^2}^2\leq\mathcal{E}\left(\phi^{k-1},\phi^{k}\right),\quad \textit{(nCH equation)}. \tag{2.25}$$

Also note that the remainder term in the pseudo energy (2.23) is nonnegative. This implies that the energy is bounded by the initial energy, for any $s>0$*:* $E\left(\phi^{k+1}\right)\leq\mathcal{E}\left(\phi^{k},\phi^{k+1}\right)\leq\mathcal{E}\left(\phi^{-1},\phi^{0}\right)\equiv E\left(\phi^{0}\right)$ *by taking* $\phi^{-1}=\phi^{0}$*. Therefore, we say that the scheme is unconditionally energy stable.*

In the sequel, we will propose fully discrete versions of these schemes and provide the corresponding analysis.

2.3 | Discrete energy and the fully discrete convex splitting schemes

We begin by defining a fully discrete energy that is consistent with the energy (2.1) in continuous space. In particular, the discrete energy $F:\mathcal{C}_{m\times n}\to\mathbb{R}$ is given by

$$F(\phi):=\frac{1}{4}\left\|\phi\right\|_4^4+\frac{\gamma_c-\gamma_e}{2}\left\|\phi\right\|_2^2+\frac{[J\star\mathbf{1}]}{2}\left\|\phi\right\|_2^2-\frac{h^2}{2}\left(\phi\|\left[J\star\phi\right]\right), \tag{2.26}$$

where $J:=J_c-J_e$, and $J_\alpha\in\mathcal{V}_{m\times n}$, $\alpha=c,e$, are defined via the vertex-centered grid restrictions $(J_\alpha)_{i+\frac{1}{2},j+\frac{1}{2}}:=\mathsf{J}_\alpha(p_{i+\frac{1}{2}},p_{j+\frac{1}{2}})$.

Lemma 2.5. *Suppose that* $\phi\in\mathcal{C}_{m\times n}$ *is periodic and define*

$$F_c(\phi):=\frac{1}{4}\left\|\phi\right\|_4^4+\frac{2\left[J_c\star\mathbf{1}\right]+\gamma_c}{2}\left\|\phi\right\|_2^2, \tag{2.27}$$

$$F_e(\phi):=\frac{\left[J_c\star\mathbf{1}\right]+\left[J_e\star\mathbf{1}\right]+\gamma_e}{2}\left\|\phi\right\|_2^2+\frac{h^2}{2}\left(\phi\|\left[J\star\phi\right]\right). \tag{2.28}$$

Then F_c *and* F_e *are convex, and the gradients of the respective energies are*

$$\delta_\phi F_c=\phi^3+\left(2\left[J_c\star\mathbf{1}\right]+\gamma_c\right)\phi\,,\quad \delta_\phi F_e=\left(\left[J_c\star\mathbf{1}\right]+\left[J_e\star\mathbf{1}\right]+\gamma_e\right)\phi+\left[J\star\phi\right]. \tag{2.29}$$

Hence F, as defined in (2.26), admits the convex splitting $F=F_c-F_e$*.*

Proof. F_c is clearly convex. To see that F_e is convex, we make use of the estimate (2.12), and observe that $\frac{d^2}{ds^2}F_e(\phi+s\psi)\Big|_{s=0}\geqslant 0$, for any periodic $\psi\in\mathcal{C}_{m\times n}$. The details are suppressed for brevity. □

We now describe the fully discrete schemes in detail. The scheme can be formulated as follows: Given $\phi^k\in\mathcal{C}_{m\times n}$ periodic, find ϕ^{k+1}, $w^{k+1/2}\in\mathcal{C}_{m\times n}$ periodic so that

$$\phi^{k+1}-\phi^{k}=-Msw^{k+1/2},\quad \text{(nAC equation)}, \tag{2.30}$$

$$\phi^{k+1}-\phi^{k}=s\Delta_h w^{k+1/2},\quad \text{(nCH equation)}, \tag{2.31}$$

$$\begin{aligned}w^{k+1/2}:=\;&\eta\left(\phi^{k},\phi^{k+1}\right)+\left(2\left[J_c\star\mathbf{1}\right]+\gamma_c\right)\phi^{k+1/2}\\&-\left(\left[J_c\star\mathbf{1}\right]+\left[J_e\star\mathbf{1}\right]+\gamma_e\right)\hat{\phi}^{k+1/2}-\left[J\star\hat{\phi}^{k+1/2}\right],\end{aligned} \tag{2.32}$$

in which Δ_h is the standard 5-point discrete Laplacian operator, $\eta\left(\phi^{k},\phi^{k+1}\right)$, $\phi^{k+1/2}$, $\hat{\phi}^{k+1/2}$ are given by (2.21) and (2.22), respectively.

2.4 | Unconditional solvability and energy stability

Now, we show that the convexity splitting is translated into solvability and stability for our scheme, both (2.30) and (2.31). The basic method for the proof of the following result was established in Guan et al[48] and Guan et al[50]—see also other studies[56-58]—and we therefore omit it for brevity.

First, we present the theorem regarding the unique solvability of scheme (2.31).

Theorem 2.6. *The scheme (2.31) is discretely mass conservative, ie,* $\left(\phi^{k+1}-\phi^{k}\|\mathbf{1}\right)=0$*, for all* $k\geqslant 0$*, and uniquely solvable for any time step size* $s>0$*.*

Next, we present the discrete version of Lemma 2.3.

Lemma 2.7. *Suppose that* $\phi\in C_{m\times n}$ *is periodic and the discrete energy* F *is defined in Equation 2.26. There exists a nonnegative constant* C *such that* $F(\phi)+C\geqslant 0$*. More specifically,*

$$\frac{1}{8}\|\phi\|_4^4\leq F(\phi)+\frac{(\gamma_c-\gamma_e-2[J_e\star\mathbf{1}])^2}{2}|\Omega|, \tag{2.33}$$

$$\frac{1}{2}\|\phi\|_2^2\leq F(\phi)+\frac{(\gamma_c-\gamma_e-2[J_e\star\mathbf{1}]-1)^2}{4}|\Omega|. \tag{2.34}$$

The following result is a discrete version of Theorem 2.4; its proof can be found in Guan et al.[50]

Theorem 2.8. *Suppose the energy* $F(\phi)$ *is defined in Equation 2.26; assume* $\phi^{k+1},\ \phi^{k}\in C_{m\times n}$ *are periodic and they are solutions to the scheme (2.30) (for the nAC equation) or (2.31) (for the nCH equation). Then for any* $s>0$*,*

$$\mathcal{E}\left(\phi^{k},\phi^{k+1}\right)+Ms\left\|w^{k+1/2}\right\|_2^2\leq\mathcal{E}\left(\phi^{k-1},\phi^{k}\right),\quad \textit{(nAC equation)}, \tag{2.35}$$

$$\mathcal{E}\left(\phi^{k},\phi^{k+1}\right)+s\left\|\nabla_h w^{k+1/2}\right\|_2^2\leq\mathcal{E}\left(\phi^{k-1},\phi^{k}\right),\quad \textit{(nCH equation)}, \tag{2.36}$$

with the discrete pseudo energy $\mathcal{E}\left(\phi^{k},\phi^{k+1}\right)$ *given by*

$$\begin{aligned}\mathcal{E}\left(\phi^{k},\phi^{k+1}\right)=F\left(\phi^{k+1}\right)&+\frac{([J_c\star\mathbf{1}]+[J_e\star\mathbf{1}]+\gamma_c+\gamma_e)}{4}\left\|\phi^{k+1}-\phi^{k}\right\|_2^2\\&+\frac{h^2}{4}\left(\left[J\star\left(\phi^{k+1}-\phi^{k}\right)\right]\|\phi^{k+1}-\phi^{k}\right).\end{aligned} \tag{2.37}$$

Most importantly, the remainder term in the pseudo energy (2.37) is nonnegative. This implies that the energy is bounded by the initial energy, for any $s>0$*:* $F\left(\phi^{k+1}\right)\leq\mathcal{E}\left(\phi^{k},\phi^{k+1}\right)\leq\mathcal{E}\left(\phi^{-1},\phi^{0}\right)\equiv F\left(\phi^{0}\right)$ *by taking* $\phi^{-1}=\phi^{0}$*.*

Putting Lemma 2.7 and Theorem 2.8 together, we immediately get the following 2 results. The proof can be found in Guan et al.[48]

Corollary 2.9. *Suppose that* $\left\{\phi^{k},w^{k}\right\}_{k=1}^{l}\in[C_{m\times n}]^2$ *are a sequence of periodic solution pairs of the scheme (2.30) (for the nAC equation) or (2.31) (for the nCH equation), with the starting values* ϕ^{0}*. Then, for any* $1\leq k\leq l$*,*

$$\frac{1}{8}\left\|\phi^{k}\right\|_4^4\leq F\left(\phi^{0}\right)+\frac{(\gamma_c-\gamma_e-2[J_e\star\mathbf{1}])^2}{2}|\Omega|, \tag{2.38}$$

$$\frac{1}{2}\left\|\phi^{k}\right\|_2^2\leq F\left(\phi^{0}\right)+\frac{(\gamma_c-\gamma_e-2[J_e\star\mathbf{1}]-1)^2}{4}|\Omega|. \tag{2.39}$$

Theorem 2.10. *Suppose* $\Phi\in C_{per}^{r}(\Omega)$*, where* $r\in\mathbb{Z}^{+}$ *is sufficiently large, and set* $\phi_{i,j}^{0}:=\Phi(p_i,p_j)$*. Suppose that* $\left\{\phi^{k},w^{k}\right\}_{k=1}^{l}\in[C_{m\times n}]^2$ *are a sequence of periodic solution pairs of the scheme (2.30) (for the nAC equation) or (2.31) (for the nCH equation), with the starting values* ϕ^{0}*. There exist constants* $C_3,C_4,C_5>0$*, which are independent of* h *and* s*, such that*

$$\max_{1\leq k\leq l}\left\|\phi^{k}\right\|_4\leq C_3. \tag{2.40}$$

$$\max_{1\leq k\leq l}\left\|\phi^{k}\right\|_2\leq C_4. \tag{2.41}$$

2.5 | Convergence result in $\ell^{\infty}(\ell^{2})$ and $\ell^{\infty}(\ell^{\infty})$ norm

We conclude this subsection with the statement of local-in-time error estimates for our second-order convex splitting schemes, including both (2.30) for the nAC equation and (2.31) for the nCH equation, in 2 dimensions. The detailed proof is given in the

next 3 sections. The extension of the proofs to 3 dimensions is omitted for the sake of brevity; see Remark 5.4 for some of the details.

For the nAC equation, the existence and uniqueness of solution to the IPDE (1.2) has been studied by Bates and Fife in previous studies.[11,62] Using similar techniques, one can establish the existence and uniqueness of a smooth, periodic solution to the IPDE (1.2) with smooth periodic initial data. The second-order convergence of the scheme (2.30) for the nAC equation is stated in the following theorem.

Theorem 2.11. *Given smooth, periodic initial data $\Phi(x_1, x_2, t = 0)$, we assume that the unique, smooth, periodic solution for the nAC equation 1.1 is given by $\Phi(x, y, t)$ on Ω for $0 < t \leq T$, for some $T < \infty$. Denote $\Phi^k_{i,j} := \Phi^k(p_i, p_j)$, and set $e^k_{i,j} := \Phi^k_{i,j} - \phi^k_{i,j}$, where $\phi^k_{i,j} \in \mathcal{C}_{m\times n}$ is kth periodic solution of (2.30) with $\phi^0_{i,j} := \Phi^0_{i,j}$. Then, provided s and h are sufficiently small, we have*

$$\left\| e^l \right\|_2 \leq C \left(h^2 + s^2 \right), \tag{2.42}$$

for all positive integers l, such that $ls \leq T$, where $C > 0$ is independent of h and s.

For the nCH equation, the existence and uniqueness of a smooth, periodic solution to the IPDE (1.2) with smooth periodic initial data may be established using techniques developed by Bates and Han in previous studies.[29,30] In the following pages, we denote this IPDE solution by Φ. Motivated by the results of Bates and Han, and based on the assumptions in the introduction, the global in time L^∞ bound is available for Φ. Moreover, with certain analysis techniques, the higher order H^m (for any $m \geqslant 1$) regularity could also be derived for Φ, with local-in-time existence, and with the assumption of smooth periodic initial data. Therefore, it will be reasonable to assume that

$$\|\Phi\|_{L^\infty(0,T;L^4)} + \|\Phi\|_{L^\infty(0,T;L^\infty)} + \|\nabla\Phi\|_{L^\infty(0,T;L^\infty)} < C, \tag{2.43}$$

for any $T > 0$, and therefore also, using a consistency argument, that

$$\max_{1\leq k\leq \ell} \left\| \Phi^k \right\|_4 + \max_{1\leq k\leq \ell} \left\| \Phi^k \right\|_\infty + \max_{1\leq k\leq \ell} \left\| \nabla_h \Phi^k \right\|_\infty < C, \tag{2.44}$$

after setting $\Phi^k_{i,j} := \Phi(p_i, p_j, t_k)$, where C is independent of h and s and $t_k = k\cdot s$. The IPDE solution Φ is also mass conservative, meaning that, for all $0 \leq t \leq T$, $\int_\Omega (\Phi(\mathbf{x}, 0) - \Phi(\mathbf{x}, t))\, d\mathbf{x} = 0$. For our numerical scheme, on choosing $\phi^0_{i,j} := \Phi^0_{i,j}$, we note that $\left(\phi^k - \Phi^0 \| \mathbf{1}\right) = 0$, for all $k \geqslant 0$. But, unfortunately, $\left(\phi^k - \Phi^k \| \mathbf{1}\right) \neq 0$ in general. On the other hand, by consistency,

$$\beta(t) = \int_\Omega \Phi(\mathbf{x}, t) d\mathbf{x} - \frac{1}{L_1 L_2} h^2 \left(\Phi(t) \| \mathbf{1}\right) - \left(\int_\Omega \Phi^0(\mathbf{x}) d\mathbf{x} - \frac{1}{L_1 L_2} h^2 \left(\Phi^0 \| \mathbf{1}\right) \right), \tag{2.45}$$

for some $C > 0$ that is independent of k and h. A more detailed consistency analysis shows that $|\beta(t)| \leq Ch^2$, $\forall t \geqslant 0$, and the estimates for all its higher order derivatives are available. Then we have

$$\frac{1}{L_1 L_2} h^2 \left(\phi^k - \Phi^k \| \mathbf{1}\right) =: \beta^k = \beta\left(t^k\right), \quad \left|\beta^k\right| \leq Ch^2, \tag{2.46}$$

for all $1 \leq k \leq l$. We set $\tilde{\Phi}(\cdot, t) := \Phi(\cdot, t) + \beta(t)$ and observe $\left(\phi^k - \tilde{\Phi}^k \| \mathbf{1}\right) = 0$ and also

$$\max_{1\leq k\leq \ell} \left\| \tilde{\Phi}^k \right\|_4 + \max_{1\leq k\leq \ell} \left\| \tilde{\Phi}^k \right\|_\infty + \max_{1\leq k\leq \ell} \left\| \nabla_h \tilde{\Phi}^k \right\|_\infty < C. \tag{2.47}$$

Finally, the assumptions on the continuous kernel J, specifically (2.5), and the consistency of the discrete convolution imply that $[J_c \star \mathbf{1}] + \gamma_c - [J_e \star \mathbf{1}] - \gamma_e > 0$. Furthermore, we make the following assumption to simplify the convergence analysis:

$$B_c = 2\,[J_c \star \mathbf{1}] + \gamma_c, \quad B_e = [J_c \star \mathbf{1}] + [J_e \star \mathbf{1}] + \gamma_e, \quad \text{and } B_c - 3B_e = \alpha_0 > 0, \tag{2.48}$$

for some α_0 that is independent of h, provided that h is sufficiently small. However, numerical evidence indicates that our scheme converges at the same rate when $\alpha_0 \leq 0$.

Theorem 2.12. *Given smooth, periodic initial data $\Phi(x_1, x_2, t = 0)$, suppose the unique, smooth, periodic solution for the IPDE (1.2) is given by $\Phi(x, y, t)$ on Ω for $0 < t \leq T$, for some $T < \infty$. Define $\Phi^k_{i,j}$ as above and set $e^k_{i,j} := \Phi^k_{i,j} - \phi^k_{i,j}$, where $\phi^k_{i,j} \in \mathcal{C}_{m\times n}$ is kth periodic solution of (2.31) with $\phi^0_{i,j} := \Phi^0_{i,j}$. Then, provided s and h are sufficiently small with the linear refinement path constraint $s \leq Ch$, with C any fixed constant, we have*

$$\left\| e^l \right\|_2 \le C \left(h^2 + s^2 \right), \tag{2.49}$$

for all positive integers l, such that ls ≤ T, where C > 0 is independent of h and s.

Theorem 2.13. *Under the assumptions of Theorem 2.12, we also have optimal order convergence of the numerical solution of the scheme (2.31) in the ℓ^∞ norm. Namely, if s and h are sufficiently small, for all positive integers l, such that ls ≤ T, we have*

$$\left\| e^l \right\|_\infty \le C \left(h^2 + s^2 \right), \tag{2.50}$$

where C > 0 is independent of h and s.

3 | THE SECOND-ORDER CONVERGENCE ANALYSIS FOR THE NAC EQUATION

In this section, we provide a proof of Theorem 2.11. For the exact solution Φ of the nAC equation 1.1, a detailed Taylor expansion, combined with a careful Fourier analysis, indicates the following consistency estimate:

$$\Phi^{k+1} - \Phi^k = -Ms \left(\eta \left(\Phi^k, \Phi^{k+1} \right) + B_c \Phi^{k+1/2} - B_e \hat{\Phi}^{k+1/2} - \left[J \star \hat{\Phi}^{k+1/2} \right] \right) + s\tau^{k+1}, \tag{3.1}$$

$$\text{with} \quad \Phi^{k+1/2} = \frac{1}{2} \left(\Phi^k + \Phi^{k+1} \right), \ \hat{\Phi}^{k+1/2} = \frac{3}{2} \Phi^k - \frac{1}{2} \Phi^{k-1}, \tag{3.2}$$

with the local truncation error

$$\left| \tau_{i,j}^{k+1} \right| \le C_5 \left(h^2 + s^2 \right), \quad \forall i, j, k, \tag{3.3}$$

and the constant C_5 depends only on T, L_1, and L_2.

We consider the following error function, at a pointwise level:

$$e_{i,j}^k := \Phi_{i,j}^k - \phi_{i,j}^k. \tag{3.4}$$

In turn, subtracting (2.30) from (3.1) leads to

$$\begin{aligned} e^{k+1} - e^k = -Ms \big(& \eta \left(\Phi^k, \Phi^{k+1} \right) - \eta \left(\phi^k, \phi^{k+1} \right) + B_c e^{k+1/2} - B_e \hat{\mathrm{e}}^{k+1/2} \\ & - \left[J \star \hat{\mathrm{e}}^{k+1/2} \right] \big) + s\tau_{i,j}^k, \\ \text{with} \quad e^{k+1/2} = \frac{1}{2} \left(e^k + e^{k+1} \right), & \ \hat{\mathrm{e}}^{k+1/2} = \frac{3}{2} e^k - \frac{1}{2} e^{k-1}. \end{aligned} \tag{3.5}$$

Taking a discrete inner-product with (3.5) by $2e^{k+1/2} = (e^{k+1} + e^k)$, summing over i and j implies that

$$\begin{aligned} & \|e^{k+1}\|_2^2 - \|e^k\|_2^2 + 2B_c s \|e^{k+1/2}\|_2^2 + 2h^2 s \left(\eta(\Phi^k, \Phi^{k+1}) - \eta(\phi^k, \phi^{k+1}) \middle\| e^{k+1/2} \right) \\ & \le 2sh^2 \left(\tau^{k+1} \middle\| e^{k+1/2} \right) + 2B_e s h^2 \left(\hat{\mathrm{e}}^{k+1/2} \middle\| e^{k+1/2} \right) + 2h^2 s \left(\left[J \star \hat{\mathrm{e}}^{k+1/2} \right] \middle\| e^{k+1/2} \right). \end{aligned} \tag{3.6}$$

The term associated with the local truncation error could be bounded with an application of Cauchy inequality:

$$2h^2 \left(\tau^{k+1} \middle\| e^{k+1/2} \right) \le \|\tau^{k+1}\|_2^2 + \|e^{k+1/2}\|_2^2 \le \|\tau^{k+1}\|_2^2 + \frac{1}{2} (\|e^{k+1}\|_2^2 + \|e^k\|_2^2). \tag{3.7}$$

The concave term could be bounded in a straightforward way:

$$\begin{aligned} 2B_e h^2 \left(\hat{\mathrm{e}}^{k+1/2} \middle\| e^{k+1/2} \right) & \le B_e (\|\hat{\mathrm{e}}^{k+1/2}\|_2^2 + \|e^{k+1/2}\|_2^2) \\ & \le \frac{B_e}{2} (\|e^{k+1}\|_2^2 + 10\|e^k\|_2^2 + \|e^{k-1}\|_2^2). \end{aligned} \tag{3.8}$$

The term associated with the convolution could be analyzed with the help of (2.12):

$$\begin{aligned} 2h^2\left(\left[J\star\hat{\mathfrak{e}}^{k+1/2}\right]\Big\|e^{k+1/2}\right) &\le B_J(\|\hat{\mathfrak{e}}^{k+1/2}\|_2^2+\|e^{k+1/2}\|_2^2)\\ &\le \frac{B_J}{2}(\|e^{k+1}\|_2^2+10\|e^k\|_2^2+\|e^{k-1}\|_2^2), \end{aligned} \tag{3.9}$$

with $B_J=[J_c\star\mathbf{1}]+[J_e\star\mathbf{1}]$.

The rest work is focused on the analysis for the term associated with the nonlinear error. We begin with the following decomposition:

$$\begin{aligned} &\eta(\Phi^k,\Phi^{k+1})-\eta(\phi^k,\phi^{k+1})=\mathcal{NLE}_1+\mathcal{NLE}_2+\mathcal{NLE}_3,\quad \text{with}\\ &\mathcal{NLE}_1=\frac{1}{2}((\phi^{k+1})^2+(\phi^k)^2)e^{k+1/2},\quad \mathcal{NLE}_2=\frac{1}{4}(\Phi^{k+1}+\phi^{k+1})(\Phi^{k+1}+\Phi^k)e^{k+1},\\ &\mathcal{NLE}_3=\frac{1}{4}(\Phi^k+\phi^k)(\Phi^{k+1}+\Phi^k)e^k. \end{aligned} \tag{3.10}$$

The following estimate is available for the term associated with $\mathcal{NLE}_1$:

$$-2h^2\left(\mathcal{NLE}_1\Big\|e^{k+1/2}\right)\le -h^2\left((\phi^{k+1})^2\Big\|(e^{k+1/2})^2\right)-h^2\left((\phi^k)^2\Big\|(e^{k+1/2})^2\right). \tag{3.11}$$

For the term associated with $\mathcal{NLE}_2$, we have

$$\begin{aligned} 2h^2\left(\frac{1}{4}\Phi^{k+1}(\Phi^{k+1}+\Phi^k)e^{k+1}\Big\|e^{k+1/2}\right)&\le\frac{1}{2}\|\Phi^{k+1}\|_\infty(\|\Phi^{k+1}\|_\infty+\|\Phi^k\|_\infty)\|e^{k+1}\|_2\cdot\|e^{k+1/2}\|_2\\ &\le C\|e^{k+1}\|_2\cdot\|e^{k+1/2}\|_2\le C(\|e^{k+1}\|_2^2+\|e^k\|_2^2), \end{aligned} \tag{3.12}$$

$$\begin{aligned} 2h^2\left(\frac{1}{4}\phi^{k+1}(\Phi^{k+1}+\Phi^k)e^{k+1}\Big\|e^{k+1/2}\right)&=\frac{1}{2}h^2\left((\Phi^{k+1}+\Phi^k)e^{k+1}\|\phi^{k+1}e^{k+1/2}\right)\\ &\le\frac{1}{2}(\|\Phi^{k+1}\|_\infty+\|\Phi^k\|_\infty)\|e^{k+1}\|_2\cdot\|\phi^{k+1}e^{k+1/2}\|_2\le C\|e^{k+1}\|_2\cdot\|\phi^{k+1}e^{k+1/2}\|_2\\ &\le C\|e^{k+1}\|_2^2+\|\phi^{k+1}e^{k+1/2}\|_2=C\|e^{k+1}\|_2^2+h^2\left((\phi^{k+1})^2\Big\|(e^{k+1/2})^2\right), \end{aligned} \tag{3.13}$$

with the Cauchy inequality applied in the last step. Consequently, we arrive at

$$-2h^2\left(\mathcal{NLE}_2\Big\|e^{k+1/2}\right)\le C(\|e^{k+1}\|_2^2+\|e^k\|_2^2)+h^2\left((\phi^{k+1})^2\Big\|(e^{k+1/2})^2\right). \tag{3.14}$$

The estimate for the term associated with $\mathcal{NLE}_3$ is similar; the details are left to the interested readers:

$$-2h^2\left(\mathcal{NLE}_3\Big\|e^{k+1/2}\right)\le C(\|e^{k+1}\|_2^2+\|e^k\|_2^2)+h^2\left((\phi^k)^2\Big\|(e^{k+1/2})^2\right). \tag{3.15}$$

In turn, a combination of (3.11), (3.14), and (3.15) into (3.10) yields the inner-product associated with the nonlinear error:

$$-2h^2\left(\eta(\Phi^k,\Phi^{k+1})-\eta(\phi^k,\phi^{k+1})\Big\|e^{k+1/2}\right)\le C(\|e^{k+1}\|_2^2+\|e^k\|_2^2). \tag{3.16}$$

Finally, a substitution of (3.7) to (3.9) and (3.16) into (3.6) indicates that

$$\|e^{k+1}\|_2^2-\|e^k\|_2^2+2B_cs\|e^{k+1/2}\|_2^2\le Cs(\|e^{k+1}\|_2^2+\|e^k\|_2^2+\|e^{k-1}\|_2^2)+s\|\tau^{k+1}\|_2^2. \tag{3.17}$$

The application of discrete Gronwall inequality implies the $\ell^\infty(0,T;\ell^2)$ convergence estimate (2.42), using the local truncation error bound (3.3). The proof of Theorem 2.11 is complete.

Remark 3.1. In the convergence proof for Theorem 2.11, the decomposition (3.10) has played a key role in the nonlinear error estimates. Because of the well-posed nonlinear inner-product in (3.11), the degree of nonlinearity of the 2 other nonlinear inner-products could be perfectly controlled, with only the maximum norm bound of the exact solution Φ needed.

As a result of this technique, an estimate for the maximum norm of the numerical solution is avoided, which usually has to be obtained in the nonlinear convergence analysis. Because of this fact, an inverse inequality is not needed in the presented

analysis, and the $\ell^\infty(0,T;\ell^2)$ convergence for the nAC equation turns out to be unconditional, ie, no scaling law between the time step size s and the grid size h is required for the desired convergence result.

Remark 3.2. We also observe that the technical assumption (2.48) (for the physical parameters) is not required in the convergence analysis for the nAC equation.

4 | HIGHER ORDER CONSISTENCY ANALYSIS OF (2.31) FOR THE NCH EQUATION: ASYMPTOTIC EXPANSION OF THE NUMERICAL SOLUTION

For simplicity of presentation, we denote

$$\tilde{\Phi}^{k+1/2} = \frac{1}{2}\left(\tilde{\Phi}^k + \tilde{\Phi}^{k+1}\right), \quad \hat{\tilde{\Phi}}^{k+1/2} = \frac{3}{2}\tilde{\Phi}^k - \frac{1}{2}\tilde{\Phi}^{k-1}. \tag{4.1}$$

By consistency, the IPDE solution $\tilde{\Phi}$ solves the discrete equation

$$\tilde{\Phi}^{k+1} - \tilde{\Phi}^k = s\Delta_h\left(\eta\left(\tilde{\Phi}^k, \tilde{\Phi}^{k+1}\right) + B_c\tilde{\Phi}^{k+1/2} - B_e\hat{\tilde{\Phi}}^{k+1/2} - \left[J \star \hat{\tilde{\Phi}}^{k+1/2}\right]\right) + s\tau^{k+1}, \tag{4.2}$$

where the local truncation error τ^{k+1} satisfies

$$\left|\tau_{i,j}^{k+1}\right| \le C_6\left(h^2 + s^2\right), \tag{4.3}$$

for all i, j, and k for some $C_6 \geqslant 0$ that depends only on T, L_1, and L_2.

Meanwhile, it is observed that the leading local truncation error in (4.2) will not be enough to recover an a priori $W^{1,\infty}$ bound for the numerical solution, needed in the stability and convergence analysis. To remedy this, we use a higher order consistency analysis, via a perturbation argument, to recover such a bound in later analysis. In more detail, we need to construct supplementary fields, Φ_h^1, Φ_s^1, and $\check{\Phi}$, satisfying

$$\check{\Phi} = \tilde{\Phi} + h^2\Phi_{h,1} + s^2\Phi_{s,1}, \tag{4.4}$$

so that a higher $O(s^3 + h^4)$ consistency is satisfied with the given numerical scheme (2.31). The constructed fields $\Phi_{h,1}$, $\Phi_{s,1}$, which will be found using a perturbation expansion, will depend solely on the exact solution Φ.

The following truncation error analysis for the spatial discretization can be obtained by using a straightforward Taylor expansion for the exact solution:

$$\partial_t\tilde{\Phi} = \Delta_h\left(\tilde{\Phi}^3 + \left([J \star \mathbf{1}] + \gamma_c - \gamma_e\right)\tilde{\Phi} - \left[J \star \tilde{\Phi}\right]\right) + h^2\boldsymbol{g}^{(0)} + O(h^4), \quad \forall\,(i,j). \tag{4.5}$$

Here the spatially discrete function $\boldsymbol{g}^{(0)}$ is smooth enough in the sense that its discrete derivatives are bounded. Also note that there is no $O(h^3)$ truncation error term, because the centered difference used in the spatial discretization gives local truncation errors with only even order terms, $O(h^2)$, $O(h^4)$, etc.

The spatial correction function $\Phi_{h,1}$ is given by solving the following equation:

$$\partial_t\Phi_{h,1} = \Delta_h\left(3\tilde{\Phi}^2\Phi_{h,1} + \left([J \star \mathbf{1}] + \gamma_c - \gamma_e\right)\Phi_{h,1} - \left[J \star \Phi_{h,1}\right]\right) - \boldsymbol{g}^{(0)}, \quad \forall\,(i,j). \tag{4.6}$$

Existence of a solution of the above linear system of ODEs is a standard exercise. Note that the solution depends only on the exact solution, Φ. In addition, the divided differences of $\Phi_{h,1}$ of various orders are bounded.

Now, we define

$$\Phi_h^* := \tilde{\Phi} + h^2\Phi_{h,1}. \tag{4.7}$$

A combination of (4.5) and (4.6) leads to the fourth-order local truncation error for Φ_h^*:

$$\partial_t\Phi_h^* = \Delta_h\left(\left(\Phi_h^*\right)^3 + \left([J \star \mathbf{1}] + \gamma_c - \gamma_e\right)\Phi_h^* - \left[J \star \Phi_h^*\right]\right) + O(h^4), \quad \forall\,(i,j), \tag{4.8}$$

for which the following estimate was used:

$$\left(\Phi_h^*\right)^3 = \left(\tilde{\Phi} + h^2\Phi_{h,1}\right)^3 = \tilde{\Phi}^3 + 3h^2\tilde{\Phi}^2\Phi_{h,1} + O(h^4). \tag{4.9}$$

We remark that the above derivation is valid since all $O(h^2)$ terms cancel in the expansion.

Regarding the temporal correction term, we observe that the application of the second-order convex splitting scheme (2.31) for the profile Φ_h^* gives

$$\begin{aligned}\frac{\left(\Phi_h^*\right)^{k+1}-\left(\Phi_h^*\right)^k}{s}&=\Delta_h\left(\eta\left((\Phi_h^*)^k,(\Phi_h^*)^{k+1}\right)+B_c\left(\Phi_h^*\right)^{k+1/2}-B_e\hat{\Phi}_h^{*\,k+1/2}\right.\\&\quad\left.-\left[J\star\hat{\Phi}_h^{*\,k+1/2}\right]\right)+s^2\boldsymbol{h}^{(1)}+O(s^3)+O(h^4),\quad\forall\,(i,j),\\&\text{with}\quad\left(\Phi_h^*\right)^{k+1/2}=\frac{1}{2}\left(\left(\Phi_h^*\right)^k+\left(\Phi_h^*\right)^{k+1}\right),\ \ \hat{\Phi}_h^{*\,k+1/2}=\frac{3}{2}\left(\Phi_h^*\right)^k-\frac{1}{2}\left(\Phi_h^*\right)^{k-1},\end{aligned}\tag{4.10}$$

at any grid point (i,j). In turn, the first-order temporal correction function $\Phi_{s,1}$ is given by the solution of the following system of linearized ordinary differential equations

$$\partial_t\Phi_{s,1}=\Delta_h(3\left(\Phi_h^*\right)^2\Phi_{s,1}+([J_c\star\mathbf{1}]-[J_e\star\mathbf{1}]+\gamma_c-\gamma_e)\,\Phi_{s,1}-\left[J\star\Phi_{s,1}\right])-\boldsymbol{h}^{(1)}.\tag{4.11}$$

Again, the solution of (4.11), which exists and is unique, depends solely on the profile Φ_h^* and is smooth enough in the sense that its divided differences of various orders are bounded. Similar to (4.10), an application of the second-order convex splitting scheme to $\Phi_{s,1}$ reads

$$\begin{aligned}\frac{\left(\Phi_{s,1}\right)^{k+1}-\left(\Phi_{s,1}\right)^k}{s}&=\Delta_h\left(\frac{1}{2}\left((\Phi_h^*)^k+(\Phi_h^*)^{k+1}\right)\left((\Phi_h^*)^k\Phi_{s,1}^k+(\Phi_h^*)^{k+1}\Phi_{s,1}^{k+1}\right)\right.\\&\quad+\frac{1}{4}\left(\Phi_{s,1}^k+\Phi_{s,1}^{k+1}\right)\left(\left((\Phi_h^*)^k\right)^2+\left((\Phi_h^*)^{k+1}\right)^2\right)\\&\quad\left.+B_c\Phi_{s,1}^{k+1}-B_e\hat{\Phi}_{s,1}^{\,k+1/2}-\left[J\star\hat{\Phi}_{s,1}^{\,k+1/2}\right]\right)\\&\quad-(\boldsymbol{h}^{(1)})^k+s(\boldsymbol{h}^{(2)})^k+O(s^2)+O(sh^2),\quad\forall\,(i,j),\\&\text{with}\quad\Phi_{s,1}^{k+1/2}=\frac{1}{2}\left(\Phi_{s,1}^k+\Phi_{s,1}^{k+1}\right),\ \hat{\Phi}_{s,1}^{\,k+1/2}=\frac{3}{2}\Phi_{s,1}^k-\frac{1}{2}\Phi_{s,1}^{k-1}.\end{aligned}\tag{4.12}$$

Therefore, a combination of (4.10) and (4.12) shows that

$$\begin{aligned}\frac{\breve{\Phi}^{k+1}-\breve{\Phi}^k}{s}&=\Delta_h\left(\eta\left(\breve{\Phi}^k,\breve{\Phi}^{k+1}\right)+B_c\breve{\Phi}^{k+1/2}-B_e\hat{\breve{\Phi}}^{\,k+1/2}\right.\\&\quad\left.-\left[J\star\hat{\breve{\Phi}}^{\,k+1/2}\right]\right)+O(s^3+s^3h^2+h^4),\quad\forall\,(i,j),\\&\text{with}\quad\breve{\Phi}^{k+1/2}=\frac{1}{2}\left(\breve{\Phi}^k+\breve{\Phi}^{k+1}\right),\ \hat{\breve{\Phi}}^{\,k+1/2}=\frac{3}{2}\breve{\Phi}^k-\frac{1}{2}\breve{\Phi}^{k-1},\end{aligned}\tag{4.13}$$

in which the construction (4.4) for the approximate solution $\breve{\Phi}$ is recalled and we have used the following estimate

$$\begin{aligned}&\eta\left(\breve{\Phi}^k,\breve{\Phi}^{k+1}\right)=\eta\left((\Phi_h^*)^k+s^2\Phi_{s,1}^k,(\Phi_h^*)^{k+1}+s^2\Phi_{s,1}^{k+1}\right)\\&=\eta\left((\Phi_h^*)^k,(\Phi_h^*)^{k+1}\right)+\frac{1}{2}s^2\left((\Phi_h^*)^k+(\Phi_h^*)^{k+1}\right)\left((\Phi_h^*)^k\Phi_{s,1}^k+(\Phi_h^*)^{k+1}\Phi_{s,1}^{k+1}\right)\\&\quad+\frac{1}{4}s^2\left(\Phi_{s,1}^k+\Phi_{s,1}^{k+1}\right)\left(\left((\Phi_h^*)^k\right)^2+\left((\Phi_h^*)^{k+1}\right)^2\right)+O(s^4).\end{aligned}\tag{4.14}$$

Remark 4.1. Trivial initial data $\Phi_{h,1}(\cdot,t=0)\equiv 0$, $\Phi_{s,1}(\cdot,t=0)\equiv 0$ are given to $\Phi_{h,1}$ and $\Phi_{s,1}$ as (4.6) and (4.11), respectively. Thus, we conclude that

$$\phi^0\equiv\breve{\Phi}^0,\qquad\left(\phi^k-\breve{\Phi}^k\|\mathbf{1}\right)=0,\quad\forall k\geqslant 0.\tag{4.15}$$

These 2 properties will be used in later analysis.

Remark 4.2. The reason for such a higher order asymptotic expansion and truncation error estimate is to justify an a priori $W^{1,\infty}$ bound of the numerical solution, which is needed in the H^{-1} convergence analysis. In more detail, in the expansion for the discrete gradient of the nonlinear error term and its H^{-1} inner-product estimate with the error function, an a priori $W^{1,\infty}$ bound of the numerical solution at a discrete level is needed to control the ℓ^2 error of the numerical solution. To obtain such a bound, we have to perform a higher order consistency analysis, up to $O(s^3+h^4)$, instead of the leading $O(s^2+h^2)$ consistency for the exact solution, through a construction of approximate solution that satisfies the numerical scheme with higher order accuracy. In turn, an $O(s^3 + h^4)$ convergence in $\ell^\infty(0, T; \ell^2)$ norm can be derived, between the numerical solution and the constructed approximate solution, and this convergence result is used to recover the a priori $W^{1,\infty}$ assumption for the numerical solution, under a mild linear refinement constraint, $s \le Ch$, with the help of inverse inequality.

5 | CONVERGENCE PROOF FOR THE NCH EQUATION

As stated earlier, the purpose of the higher order expansion (4.4) is to obtain a $W^{1,\infty}$ bound of the error function via its L^2 norm in higher order accuracy by using an inverse inequality in spatial discretization, which will be shown below. A detailed analysis shows that

$$\left\|\check{\Phi}-\Phi\right\|_\infty+\left\|\nabla_h\left(\check{\Phi}-\Phi\right)\right\|_\infty\le C(s^2+h^2), \tag{5.1}$$

since $\left\|\Phi_{h,1}\right\|_\infty, \left\|\nabla_h\Phi_{h,1}\right\|_\infty, \left\|\Phi_{s,1}\right\|_\infty, \left\|\nabla_h\Phi_{s,1}\right\|_\infty \le C$. Subsequently, the following error function is considered:

$$\check{e}^k_{i,j} := \check{\Phi}^k_{i,j} - \phi^k_{i,j}. \tag{5.2}$$

In other words, instead of a direct comparison between the numerical solution ϕ and the exact solution Φ (or $\tilde{\Phi}$), we estimate the error between the numerical solution and the constructed solution to obtain a higher order convergence in the $\|\cdot\|_2$ norm, which follows the technique originally proposed in Strang.[63] Subtracting (2.31) from (4.13) yields

$$\begin{aligned}\check{e}^{k+1}-\check{e}^k = s\Delta_h\Big(&\eta\left(\check{\Phi}^k,\check{\Phi}^{k+1}\right)-\eta\left(\phi^k,\phi^{k+1}\right)+B_c\check{e}^{k+1/2}-B_e\hat{\check{e}}^{k+1/2}\\&-\left[J\star\hat{\check{e}}^{k+1/2}\right]\Big)+s\hat{\tau}^k_{i,j},\quad \left|\hat{\tau}^k_{i,j}\right|\le C(s^3+h^4),\\ \text{with}\quad \check{e}^{k+1/2}=\frac{1}{2}\left(\check{e}^k+\check{e}^{k+1}\right),\ &\hat{\check{e}}^{k+1/2}=\frac{3}{2}\check{e}^k-\frac{1}{2}\check{e}^{k-1}.\end{aligned} \tag{5.3}$$

5.1 | Preliminary error estimates for linear terms

Proposition 5.1. *We have*

$$-2h^2\left(\left[J\star\hat{\check{e}}^{k+1/2}\right]\left\|\Delta_h\check{e}^{k+1/2}\right)\le\frac{C_7}{\alpha}\left(\left\|\check{e}^k\right\|_2^2+\left\|\check{e}^{k-1}\right\|_2^2\right)+\alpha\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^2,\quad\forall\alpha>0, \tag{5.4}$$

$$-2h^2\left(\hat{\check{e}}^{k+1/2}\left\|\Delta_h\check{e}^{k+1/2}\right)\le-\left(\left\|\nabla_h\check{e}^{k+1}\right\|_2^2-\left\|\nabla_h\check{e}^k\right\|_2^2\right)+5\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^2+\left\|\nabla_h\check{e}^{k-1/2}\right\|_2^2. \tag{5.5}$$

Proof. The first inequality (5.4) is a direct application of Lemma 2.2 and Cauchy inequality:

$$\begin{aligned}-2h^2\left(\left[J\star\hat{\check{e}}^{k+1/2}\right]\left\|\Delta_h\check{e}^{k+1/2}\right)&\le\frac{sC_2}{\alpha}\left\|\hat{\check{e}}^{k+1/2}\right\|_2^2+\alpha\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^2\\&\le\frac{C_2}{\alpha}\left(3\left\|\check{e}^k\right\|_2^2+\left\|\check{e}^{k-1}\right\|_2^2\right)+\alpha\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^2.\end{aligned} \tag{5.6}$$

For the second inequality (5.5), we start from the summation by parts:

$$-2h^2\left(\hat{\check{e}}^{k+1/2}\left\|\Delta_h\check{e}^{k+1/2}\right)=2h^2\left(\nabla_h\hat{\check{e}}^{k+1/2}\left\|\nabla_h\check{e}^{k+1/2}\right)=h^2\left(\nabla_h\hat{\check{e}}^{k+1/2}\left\|\nabla_h\left(\check{e}^k+\check{e}^{k+1}\right)\right)\right. . \tag{5.7}$$

Meanwhile, the term $\hat{\check{e}}^{k+1/2}$ can be rewritten as

$$\hat{\check{e}}^{k+1/2} = \frac{3}{2}\check{e}^{k} - \frac{1}{2}\check{e}^{k-1} = -\left(\check{e}^{k+1} - \check{e}^{k}\right) + 2\check{e}^{k+1/2} - \check{e}^{k-1/2}, \tag{5.8}$$

which in turn gives the following estimate:

$$\begin{aligned}
&2h^2\left(\nabla_h\hat{\check{e}}^{k+1/2}\middle\|\nabla_h\check{e}^{k+1/2}\right)\\
&= -h^2\left(\nabla_h\left(\check{e}^{k+1}-\check{e}^{k}\right)\middle\|\nabla_h\left(\check{e}^{k+1}+\check{e}^{k}\right)\right) + 4\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^2 - 2h^2\left(\nabla_h\check{e}^{k+1/2}\middle\|\nabla_h\check{e}^{k-1/2}\right)\\
&= -\left(\left\|\nabla_h\check{e}^{k+1}\right\|_2^2 - \left\|\nabla_h\check{e}^{k}\right\|_2^2\right) + 4\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^2 - 2h^2\left(\nabla_h\check{e}^{k+1/2}\middle\|\nabla_h\check{e}^{k-1/2}\right)\\
&\le -\left(\left\|\nabla_h\check{e}^{k+1}\right\|_2^2 - \left\|\nabla_h\check{e}^{k}\right\|_2^2\right) + 5\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^2 + \left\|\nabla_h\check{e}^{k-1/2}\right\|_2^2.
\end{aligned} \tag{5.9}$$

Finally, its combination with (5.7) results in (5.5). The proof of Proposition 5.1 is complete. □

5.2 | Preliminary nonlinear error estimates

The $W^{1,\infty}$ bound for the constructed approximate solution $\check{\Phi}$ is guaranteed by the regularity of the exact solution Φ (and henceforth $\tilde{\Phi}$ and the correction terms $\Phi_{h,1}$, $\Phi_{s,1}$), at any time step. Similarly, its divided difference in time is also bounded pointwise, which comes from the regularity in time for the constructed solution. For the numerical solution ϕ, its global in time ℓ^4 has been derived in Theorem 2.10. Moreover, to carry out the error estimate for the nonlinear term, we need to make an a priori $W^{1,\infty}$ assumption for the numerical solution at time step t^k and use the $O(s^3 + h^4)$ order convergence in ℓ^2 to recover such an assumption at the next time step t^{k+1}.

Proposition 5.2. *Suppose $\phi^j,\ \check{\Phi}^j \in C_{m\times n}$, are periodic with equal means, ie, $\left(\phi^j - \check{\Phi}^j\|\mathbf{1}\right) = 0$, $j = k, k+1$, and satisfying*

$$\left\|\check{\Phi}^k\right\|_4 + \left\|\check{\Phi}^k\right\|_\infty + \left\|\nabla_h\check{\Phi}^k\right\|_\infty + \left\|\check{\Phi}^{k+1}\right\|_4 + \left\|\check{\Phi}^{k+1}\right\|_\infty + \left\|\nabla_h\check{\Phi}^{k+1}\right\|_\infty \le C_0, \tag{5.10}$$

$$\left\|\frac{\check{\Phi}^{k+1}-\check{\Phi}^k}{s}\right\|_\infty \le C_0, \tag{5.11}$$

$$\left\|\phi^k\right\|_4 \le C_0, \quad \left\|\phi^{k+1}\right\|_4 \le C_0, \tag{5.12}$$

$$\left\|\phi^k\right\|_\infty + \left\|\nabla_h\phi^k\right\|_\infty \le C_0, \tag{5.13}$$

where C_0 is an s, h-independent positive constant. Then, there exists a positive constant C_1, which depends on C_0 but is independent of s and h, such that

$$\begin{aligned}
&2h^2\left(\eta\left(\check{\Phi}^k,\check{\Phi}^{k+1}\right) - \eta\left(\phi^k,\phi^{k+1}\right)\|\Delta_h\check{e}^{k+1/2}\right)\\
&\le \frac{C_1}{\alpha^3}\left(\left\|\check{e}^k\right\|_2^2 + \left\|\check{e}^{k+1}\right\|_2^2\right) + \alpha\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^2\\
&\quad + \frac{C_1}{\alpha}s^2\left\|\nabla_h\check{e}^k\right\|_2^2 + \frac{C_1}{\alpha}\left(1 + \left\|\phi^{k+1}\right\|_\infty^2\right)\left\|\check{e}^k\right\|_2^2, \quad \forall\alpha > 0.
\end{aligned} \tag{5.14}$$

Proof. For simplicity of presentation, we denote $\mathcal{NLE}^k = \eta\left(\check{\Phi}^k,\check{\Phi}^{k+1}\right) - \eta\left(\phi^k,\phi^{k+1}\right)$. A direct application of summation by parts reveals that

$$\begin{aligned}
&2h^2\left(\mathcal{NLE}^k\middle\|\Delta_h\check{e}^{k+1/2}\right) = -2h^2\left(\nabla_h\left(\mathcal{NLE}^k\right)\middle\|\nabla_h\check{e}^{k+1/2}\right) = \mathcal{NLI}_1^k + \mathcal{NLI}_2^k, \quad \text{with}\\
&\mathcal{NLI}_1^k = -2h^2\left(D_x\left(\mathcal{NLE}^k\right)\middle\|D_x\check{e}^{k+1/2}\right), \quad \mathcal{NLI}_2^k = -2h^2\left(D_y\left(\mathcal{NLE}^k\right)\middle\|D_y\check{e}^{k+1/2}\right).
\end{aligned} \tag{5.15}$$

We focus on the first term $\mathcal{NLI}_1^k$; the second term $\mathcal{NLI}_2^k$ can be analyzed in the same way. In x direction, we drop the subscript j in the grid index, just for simplicity of presentation. A detailed expansion shows that

$$\begin{aligned}
&D_x\left(\eta\left(\phi^k,\phi^{k+1}\right)\right)_{i+1/2}\\
&=\frac{1}{4h}\left(\left((\phi_{i+1}^{k+1})^2+(\phi_{i+1}^{k})^2\right)\left(\phi_{i+1}^{k+1}+\phi_{i+1}^{k}\right)-\left((\phi_{i}^{k+1})^2+(\phi_{i}^{k})^2\right)\left(\phi_{i}^{k+1}+\phi_{i}^{k}\right)\right)\\
&=\frac{1}{4h}\left((\phi_{i+1}^{k+1})^2+(\phi_{i+1}^{k})^2+(\phi_{i+1}^{k+1}+\phi_{i}^{k+1})(\phi_{i}^{k+1}+\phi_{i}^{k})\right)\left(\phi_{i+1}^{k+1}-\phi_{i}^{k+1}+\phi_{i+1}^{k}-\phi_{i}^{k}\right)\\
&\quad+\frac{1}{4h}\left(\phi_{i+1}^{k}-\phi_{i+1}^{k+1}+\phi_{i}^{k}-\phi_{i}^{k+1}\right)\left(\phi_{i}^{k+1}+\phi_{i}^{k}\right)\left(\phi_{i+1}^{k}-\phi_{i}^{k}\right)\\
&=\frac{1}{2}\left((\phi_{i+1}^{k+1})^2+(\phi_{i+1}^{k})^2+(\phi_{i+1}^{k+1}+\phi_{i}^{k+1})(\phi_{i}^{k+1}+\phi_{i}^{k})\right)D_x\phi_{i+1/2}^{k+1/2}\\
&\quad+\frac{1}{4}\left(\phi_{i+1}^{k}-\phi_{i+1}^{k+1}+\phi_{i}^{k}-\phi_{i}^{k+1}\right)\left(\phi_{i}^{k+1}+\phi_{i}^{k}\right)D_x\phi_{i+1/2}^{k}.
\end{aligned}\tag{5.16}$$

A similar expansion can be made for $D_x\left(\eta\left(\check{\Phi}^k,\check{\Phi}^{k+1}\right)\right)_{i+1/2}$. In turn, we arrive at

$$\begin{aligned}
&D_x\left(\eta\left(\check{\Phi}^k,\check{\Phi}^{k+1}\right)-\eta\left(\phi^k,\phi^{k+1}\right)\right)_{i+1/2}=\mathcal{NLE}_{1,1}^k+\mathcal{NLE}_{1,2}^k+\mathcal{NLE}_{1,3}^k+\mathcal{NLE}_{1,4}^k,\\
&\mathcal{NLE}_{1,1}^k=\frac{1}{2}\left((\phi_{i+1}^{k+1})^2+(\phi_{i+1}^{k})^2+(\phi_{i+1}^{k+1}+\phi_{i}^{k+1})(\phi_{i}^{k+1}+\phi_{i}^{k})\right)D_x\check{e}_{i+1/2}^{k+1/2},
\end{aligned}\tag{5.17}$$

$$\begin{aligned}
\mathcal{NLE}_{1,2}^k=&\frac{1}{2}\left(\left(\check{\Phi}_{i+1}^{k+1}+\phi_{i+1}^{k+1}\right)\check{e}_{i+1}^{k+1}+\left(\check{\Phi}_{i}^{k+1}+\phi_{i}^{k+1}\right)\check{e}_{i}^{k+1}\right.\\
&\left.+(\check{e}_{i+1}^{k+1}+\check{e}_{i}^{k+1})(\phi_{i}^{k+1}+\phi_{i}^{k})+(\check{\Phi}_{i+1}^{k+1}+\check{\Phi}_{i}^{k+1})(\check{e}_{i}^{k+1}+\check{e}_{i}^{k})\right)D_x\check{\Phi}_{i+1/2}^{k+1/2},
\end{aligned}\tag{5.18}$$

$$\mathcal{NLE}_{1,3}^k=\frac{1}{4}\left(\check{\Phi}_{i+1}^{k}-\check{\Phi}_{i+1}^{k+1}+\check{\Phi}_{i}^{k}-\check{\Phi}_{i}^{k+1}\right)\left(\check{\Phi}_{i}^{k+1}+\check{\Phi}_{i}^{k}\right)D_x\check{e}_{i+1/2}^{k},\tag{5.19}$$

$$\begin{aligned}
\mathcal{NLE}_{1,4}^k=&\frac{1}{4}\left(\left(\check{e}_{i+1}^{k}-\check{e}_{i+1}^{k+1}+\check{e}_{i}^{k}-\check{e}_{i}^{k+1}\right)\left(\check{\Phi}_{i}^{k+1}+\check{\Phi}_{i}^{k}\right)\right.\\
&\left.+\left(\phi_{i+1}^{k}-\phi_{i+1}^{k+1}+\phi_{i}^{k}-\phi_{i}^{k+1}\right)\left(\check{e}_{i}^{k+1}+\check{e}_{i}^{k}\right)\right)D_x\phi_{i+1/2}^{k}.
\end{aligned}\tag{5.20}$$

For the term $\mathcal{NLE}_{1,1}^k$, we observe the following estimate for the nonlinear coefficient:

$$\begin{aligned}
C_1&=(\phi_{i+1}^{k+1})^2+(\phi_{i+1}^{k})^2+(\phi_{i+1}^{k+1}+\phi_{i}^{k+1})(\phi_{i}^{k+1}+\phi_{i}^{k})\\
&=(\phi_{i+1}^{k+1})^2+(\phi_{i+1}^{k})^2+\phi_{i+1}^{k+1}\phi_{i}^{k+1}+(\phi_{i}^{k+1})^2+\phi_{i+1}^{k+1}\phi_{i}^{k}+\phi_{i}^{k+1}\phi_{i}^{k}\\
&\geqslant\frac{1}{2}\left((\phi_{i+1}^{k+1})^2+(\phi_{i}^{k+1})^2\right)+(\phi_{i+1}^{k})^2+\phi_{i+1}^{k+1}\phi_{i}^{k}+\phi_{i}^{k+1}\phi_{i}^{k}\\
&\geqslant(\phi_{i+1}^{k})^2-(\phi_{i}^{k})^2,
\end{aligned}\tag{5.21}$$

with a repeated application of Cauchy inequality in the last 2 steps. Meanwhile, the a priori assumption (5.13) for the numerical solution ϕ at time step t^k indicates that

$$-C_1\leq\left|\phi_{i+1}^{k}+\phi_{i}^{k}\right|\cdot\left|\phi_{i+1}^{k}-\phi_{i}^{k}\right|=h\left|\phi_{i+1}^{k}+\phi_{i}^{k}\right|\cdot\left|D_x\phi_{i+1/2}^{k}\right|\leq 2h\left\|\phi^k\right\|_\infty\cdot\left\|\nabla_h\phi^k\right\|_\infty\leq 2C_0^2h,\tag{5.22}$$

at a pointwise level. As a result, its combination with (5.17) implies that

$$-2h^2\left(\mathcal{NLE}_{1,1}^k\left\|D_x\check{e}^{k+1/2}\right)\leq 2C_0^2h\left\|D_x\check{e}^{k+1/2}\right\|_2^2.\tag{5.23}$$

Similar estimates can be derived for $\mathcal{NLE}_{1,3}^k$. The regularity assumption (5.10), (5.11) for the constructed approximate solution $\check{\Phi}$ shows that

$$\left|\check{\Phi}_{i+1}^{k}-\check{\Phi}_{i+1}^{k+1}\right|+\left|\check{\Phi}_{i}^{k}-\check{\Phi}_{i}^{k+1}\right|\leq 2s\left\|\frac{\check{\Phi}^{k+1}-\check{\Phi}^{k}}{s}\right\|_\infty\leq 2C_0s,\tag{5.24}$$

$$\left|\check{\Phi}_i^{k+1}+\check{\Phi}_i^{k}\right| \le \left\|\check{\Phi}^{k+1}\right\|_\infty + \left\|\check{\Phi}^{k}\right\|_\infty \le 2C_0, \quad \text{so that} \tag{5.25}$$

$$|C_3| = \left|\left(\check{\Phi}_{i+1}^{k}-\check{\Phi}_{i+1}^{k+1}+\check{\Phi}_i^{k}-\check{\Phi}_i^{k+1}\right)\left(\check{\Phi}_i^{k+1}+\check{\Phi}_i^{k}\right)\right| \le 4C_0^2 s, \tag{5.26}$$

at a pointwise level. In turn, we arrive at

$$\begin{aligned} -2h^2\left(\mathcal{NLE}_{1,3}^k\left\|D_x\check{e}^{k+1/2}\right\)\right) &\le 2C_0^2 s\left\|D_x\check{e}^{k+1/2}\right\|_2\cdot\left\|D_x\check{e}^{k}\right\|_2 \\ &\le \frac{1}{8}\alpha\left\|D_x\check{e}^{k+1/2}\right\|_2^2+\frac{8C_0^4}{\alpha}s^2\left\|D_x\check{e}^{k}\right\|_2^2. \end{aligned} \tag{5.27}$$

For the second nonlinear term $\mathcal{NLE}_{1,2}^k$, we start from a rewritten form:

$$\begin{aligned} \mathcal{NLE}_{1,2}^k &= \frac{1}{2}\Big(\left(\check{\Phi}_{i+1}^{k+1}+\phi_{i+1}^{k+1}+\phi_i^{k+1}+\phi_i^k\right)\check{e}_{i+1}^{k+1}+\left(\check{\Phi}_i^{k+1}+2\phi_i^{k+1}+\phi_i^k\right)\check{e}_i^{k+1} \\ &\quad +2(\check{\Phi}_{i+1}^{k+1}+\check{\Phi}_i^{k+1})\check{e}_i^{k+1/2}\Big)D_x\check{\Phi}_{i+1/2}^{k+1/2}, \\ &= \left(C_{2,1}\check{e}_{i+1}^{k+1/2}+C_{2,2}\check{e}_i^{k+1/2}+\frac{1}{2}C_{2,3}\check{e}_{i+1}^{k}+\frac{1}{2}C_{2,4}\check{e}_i^{k}\right)D_x\check{\Phi}_{i+1/2}^{k+1/2}, \\ \text{with}\quad & C_{2,1}=-C_{2,3}=\check{\Phi}_{i+1}^{k+1}+\phi_{i+1}^{k+1}+\phi_i^{k+1}+\phi_i^k,\quad C_{2,4}=-\left(\check{\Phi}_i^{k+1}+2\phi_i^{k+1}+\phi_i^k\right), \\ & C_{2,2}=2\check{\Phi}_i^{k+1}+\check{\Phi}_{i+1}^{k+1}+2\phi_i^{k+1}+\phi_i^k. \end{aligned} \tag{5.28}$$

For these nonlinear coefficients, it is clear that

$$\left\|C_{2,1}\right\|_4+\left\|C_{2,2}\right\|_4 \le C\left(\left\|\check{\Phi}^k\right\|_4+\left\|\check{\Phi}^{k+1}\right\|_4+\left\|\phi^k\right\|_4+\left\|\phi^{k+1}\right\|_4\right)\le CC_0, \tag{5.29}$$

$$\left\|C_{2,3}\right\|_\infty+\left\|C_{2,4}\right\|_\infty \le C\left(\left\|\check{\Phi}^k\right\|_\infty+\left\|\check{\Phi}^{k+1}\right\|_\infty+\left\|\phi^k\right\|_\infty+\left\|\phi^{k+1}\right\|_\infty\right)\le C\left(C_0+\left\|\phi^{k+1}\right\|_\infty\right), \tag{5.30}$$

in which the regularity condition (5.10) and a priori assumption (5.12) and (5.13) were repeated used in the derivation. In particular, we note that the $\|\cdot\|_4$ bound is available for both the approximate solution $\check{\Phi}$ and the numerical solution ϕ, at both time steps t^k and t^{k+1}, and the same for the $\|\cdot\|_\infty$ bound for $\check{\Phi}$. Meanwhile, in $\|\cdot\|_\infty$ norm for the numerical solution ϕ, we only have its bound at time step t^k, as an a priori assumption, and its bound at the next time step t^{k+1} has to be obtained by a higher order convergence in ℓ^2 norm via an inverse inequality, as will be shown later. As a result, an application of discrete Hölder inequality shows that

$$\begin{aligned} &-2h^2\left(\mathcal{NLE}_{1,2}^k\left\|D_x\check{e}^{k+1/2}\right\)\right) \\ &\le \left(2\left(\left\|C_{2,1}\right\|_4+\left\|C_{2,2}\right\|_4\right)\left\|\check{e}^{k+1/2}\right\|_4+\left(\left\|C_{2,3}\right\|_\infty+\left\|C_{2,4}\right\|_\infty\right)\left\|\check{e}^{k}\right\|_2\right)\left\|D_x\check{e}^{k+1/2}\right\|_2 \\ &\le \left(CC_0\left\|\check{e}^{k+1/2}\right\|_4+C\left(C_0+\left\|\phi^{k+1}\right\|_\infty\right)\left\|\check{e}^{k}\right\|_2\right)\left\|D_x\check{e}^{k+1/2}\right\|_2. \end{aligned} \tag{5.31}$$

Furthermore, a discrete Sobolev embedding in 2D gives

$$\left\|\check{e}^{k+1/2}\right\|_4 \le C\left\|\check{e}^{k+1/2}\right\|_2^{\frac{1}{2}}\cdot\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^{\frac{1}{2}},\quad \text{since}\quad \left(\check{e}^{k+1/2}\|\mathbf{1}\right)=0, \tag{5.32}$$

with C independent on h; its proof can be found in Guan et al.[48] We note that the zero-mean property of $\check{e}^{k+1/2}$ comes from (4.15). Therefore, the first part in (5.31) can be bounded by

$$CC_0\left\|\check{e}^{k+1/2}\right\|_4\cdot\left\|D_x\check{e}^{k+1/2}\right\|_2 \le M\left\|\check{e}^{k+1/2}\right\|_2^{\frac{1}{2}}\cdot\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^{\frac{3}{2}},\quad \text{with } M=CC_0. \tag{5.33}$$

In addition, we use the Young inequality

$$a\cdot b\le\frac{a^p}{p}+\frac{b^q}{q},\quad \forall\, a,b>0,\quad \frac{1}{p}+\frac{1}{q}=1, \tag{5.34}$$

with the choices $p=4$, $q=\frac{4}{3}$, $a=\left(6\alpha^{-1}\right)^{\frac{3}{4}}M\left\|\check{e}^{k+1/2}\right\|_2^{\frac{1}{2}}$, $b=\left(\frac{1}{6}\alpha\right)^{\frac{3}{4}}\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^{\frac{3}{2}}$, and get

$$\begin{aligned} CC_0\left\|\check{e}^{k+1/2}\right\|_4\cdot\left\|D_x\check{e}^{k+1/2}\right\|_2 &\le M\left\|\check{e}^{k+1/2}\right\|_2^{\frac{1}{2}}\cdot\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^{\frac{3}{2}}\\ =a\cdot b\le\frac{1}{4}a^4+\frac{3}{4}b^{\frac{4}{3}}&=\frac{1}{4}M^4\cdot\frac{(6)^3}{\alpha^3}\left\|\check{e}^{k+1/2}\right\|_2^2+\frac{\alpha}{8}\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^2. \end{aligned} \tag{5.35}$$

The bound for the second part in (5.31) can be obtained by Cauchy inequality:

$$C\left(C_0+\left\|\phi^{k+1}\right\|_\infty\right)\left\|\check{e}^k\right\|_2\left\|D_x\check{e}^{k+1/2}\right\|_2\le\frac{C\left(C_0^2+\left\|\phi^{k+1}\right\|_\infty^2\right)}{\alpha}\left\|\check{e}^k\right\|_2^2+\frac{1}{8}\alpha\left\|D_x\check{e}^{k+1/2}\right\|_2^2. \tag{5.36}$$

Consequently, a combination of (5.31), (5.35), and (5.36) yields

$$\begin{aligned} -2h^2\left(\mathcal{NLE}_{1,2}^k\left\|D_x\check{e}^{k+1/2}\right.\right)\le\frac{C_8}{\alpha^3}\left(\left\|\check{e}^k\right\|_2^2+\left\|\check{e}^{k+1}\right\|_2^2\right)+\frac{C\left\|\phi^{k+1}\right\|_\infty^2}{\alpha}\left\|\check{e}^k\right\|_2^2\\ +\frac{\alpha}{8}\left(\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^2+\left\|D_x\check{e}^{k+1/2}\right\|_2^2\right), \end{aligned} \tag{5.37}$$

with $C_8=27M^4+CC_0^2$.

The analysis for the fourth nonlinear term $\mathcal{NLE}_{1,4}^k$ is similar to that of $\mathcal{NLE}_{1,2}^k$. Its rewritten form reads as follows:

$$\begin{aligned} \mathcal{NLE}_{1,4}^k&=\frac{1}{4}\left(\left(\check{e}_{i+1}^k-\check{e}_{i+1}^{k+1}+\check{e}_i^k-\check{e}_i^{k+1}\right)\left(\check{\Phi}_i^{k+1}+\check{\Phi}_i^k\right)\right.\\ &\quad\left.+2\left(\phi_{i+1}^k-\phi_{i+1}^{k+1}+\phi_i^k-\phi_i^{k+1}\right)\check{e}_i^{k+1/2}\right)D_x\phi_{i+1/2}^k,\\ &=\left(C_{4,1}\check{e}_{i+1}^{k+1/2}+C_{4,2}\check{e}_i^{k+1/2}+C_{4,3}\check{e}_{i+1}^k+C_{4,4}\check{e}_i^k\right)D_x\check{\Phi}_{i+1/2}^{k+1/2},\\ \text{with}\quad C_{4,1}&=-\frac{1}{2}\left(\check{\Phi}_i^{k+1}+\check{\Phi}_i^k\right),\quad C_{4,2}=\frac{1}{2}\left(\phi_{i+1}^k-\phi_{i+1}^{k+1}+\phi_i^k-\phi_i^{k+1}-\check{\Phi}_i^{k+1}-\check{\Phi}_i^k\right),\\ C_{4,3}&=C_{4,4}=\frac{1}{2}\left(\check{\Phi}_i^{k+1}+\check{\Phi}_i^k\right). \end{aligned} \tag{5.38}$$

Similarly, these nonlinear coefficients can be bounded by

$$\left\|C_{4,1}\right\|_4+\left\|C_{4,2}\right\|_4\le C\left(\left\|\check{\Phi}^k\right\|_4+\left\|\check{\Phi}^{k+1}\right\|_4+\left\|\phi^k\right\|_4+\left\|\phi^{k+1}\right\|_4\right)\le CC_0, \tag{5.39}$$

$$\left\|C_{4,3}\right\|_\infty+\left\|C_{4,4}\right\|_\infty\le C\left(\left\|\check{\Phi}^k\right\|_\infty+\left\|\check{\Phi}^{k+1}\right\|_\infty\right)\le CC_0. \tag{5.40}$$

Note that for $C_{4,3}$ and $C_{4,4}$, since the numerical solution ϕ is not involved, the regularity assumption (5.10), (5.11) for the approximate solution $\check{\Phi}$ directly gives a bounded for these 2 coefficients. This also greatly simplifies the analysis below. Then we have

$$\begin{aligned} &-2h^2\left(\mathcal{NLE}_{1,4}^k\|D_x\check{e}^{k+1/2}\right)\\ &\le\left(2\left(\left\|C_{4,1}\right\|_4+\left\|C_{4,2}\right\|_4\right)\left\|\check{e}^{k+1/2}\right\|_4+\left(\left\|C_{4,3}\right\|_\infty+\left\|C_{4,4}\right\|_\infty\right)\left\|\check{e}^k\right\|_2\right)\left\|D_x\check{e}^{k+1/2}\right\|_2\\ &\le CC_0\left(\left\|\check{e}^{k+1/2}\right\|_4+\left\|\check{e}^k\right\|_2\right)\cdot\left\|D_x\check{e}^{k+1/2}\right\|_2. \end{aligned} \tag{5.41}$$

In turn, the estimates (5.32) to (5.36) are also valid; consequently, the following estimate can be derived:

$$\begin{aligned} -2h^2\left(\mathcal{NLE}_{1,4}^k\left\|D_x\check{e}^{k+1/2}\right.\right)\le\frac{C_9}{\alpha^3}\left(\left\|\check{e}^k\right\|_2^2+\left\|\check{e}^{k+1}\right\|_2^2\right)\\ +\frac{\alpha}{8}\left(\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^2+\left\|D_x\check{e}^{k+1/2}\right\|_2^2\right). \end{aligned} \tag{5.42}$$

Finally, a combination of (5.23), (5.27), (5.37), and (5.42) reveals that

$$\begin{aligned}\mathcal{NLI}_1^k &= -2h^2\left(D_x\left(\mathcal{NLE}^k\right)\left\|D_x\check{e}^{k+1/2}\right\|\right)\\ &\le \frac{C_{10}}{\alpha^3}\left(\left\|\check{e}^k\right\|_2^2+\left\|\check{e}^{k+1}\right\|_2^2\right)+\frac{C\left\|\phi^{k+1}\right\|_\infty^2}{\alpha}\left\|\check{e}^k\right\|_2^2\\ &\quad+\frac{\alpha}{4}\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^2+\frac{\alpha}{2}\left\|D_x\check{e}^{k+1/2}\right\|_2^2+\frac{8C_0^4}{\alpha}s^2\left\|D_x\check{e}^k\right\|_2^2,\end{aligned}\tag{5.43}$$

by choosing h with $2C_0^2h\le\frac{\alpha}{8}$. The analysis for $\mathcal{NLI}_2^k$ is essentially the same:

$$\begin{aligned}\mathcal{NLI}_2^k &= -2h^2\left(D_y\left(\mathcal{NLE}^k\right)\left\|D_y\check{e}^{k+1/2}\right\|\right)\\ &\le \frac{C_{10}}{\alpha^3}\left(\left\|\check{e}^k\right\|_2^2+\left\|\check{e}^{k+1}\right\|_2^2\right)+\frac{C\left\|\phi^{k+1}\right\|_\infty^2}{\alpha}\left\|\check{e}^k\right\|_2^2\\ &\quad+\frac{\alpha}{4}\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^2+\frac{\alpha}{2}\left\|D_y\check{e}^{k+1/2}\right\|_2^2+\frac{8C_0^4}{\alpha}s^2\left\|D_y\check{e}^k\right\|_2^2;\end{aligned}\tag{5.44}$$

and the details are skipped for brevity of presentation. Therefore, a combination of (5.43) and (5.44) results in (5.14). The proof of Proposition 5.2 is complete. □

Remark 5.3. In fact, for the nonlinear error term, the form of expansion and decomposition in its discrete gradient is not unique. However, the way in our decomposition (5.17) to (5.20) greatly facilitates the convergence analysis.

It is well known that the exact solution Φ and the nonlinear potential Φ^3 have a nonpositive H^{-1} inner-product, since $3\Phi^2\geqslant 0$. However, for the second-order numerical approximation $\eta\left(\phi^k,\phi^{k+1}\right)$, introduced by (2.21), its error estimate becomes much more tricky. In the decomposition (5.17), the nonlinear coefficient C_1 is proven to be "almost" nonnegative, as in (5.21), and the remainder term has an $O(h)$ bound given by (5.22), using the $W^{1,\infty}$ bound assumption for the numerical solution at t^k, as given by (5.13). This treatment assures a controlled property of the nonlinear inner-product associated with (5.17).

Moreover, since the numerical solution ϕ is involved with the nonlinear coefficient C_1 in (5.17), we could take the discrete gradient of the approximate solution Φ in the nonlinear expansion (5.18), and its $\|\cdot\|_\infty$ norm is directly bounded by (5.10). If it is replaced by the discrete gradient of the numerical solution, a numerical analysis is not feasible, since a bound for $\left\|\phi^{k+1}\right\|_\infty$ is not available at time step t^{k+1}.

Meanwhile, in the nonlinear expansion (5.20), an appearance of the discrete gradient of the numerical solution at time step t^k does not cause any theoretical trouble, since we have had an a priori bound (5.13), which is to be recovered by an $O(s^3+h^4)$ convergence analysis in ℓ^2 norm.

For the nonlinear errors appearing in (5.18) and (5.20), we have to rewrite them in terms of a nonlinear combination of $\check{e}^{k+1/2}$ and $\check{e}^k$. The reason is that we only have a well-posed diffusion term of $\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^2$; a positive diffusion term in either the form of $\left\|\nabla_h\check{e}^k\right\|_2^2$ or $\left\|\nabla_h\check{e}^{k+1}\right\|_2^2$ is not available in the numerical analysis, because of the second-order numerical approximation. With such a rewriting, the terms involving $\check{e}^{k+1/2}$ only require an ℓ^4 bound for the numerical and approximate solutions, given by (5.29), and the ℓ^4 estimate for $\check{e}^{k+1/2}$ is obtained by (5.32), a discrete Sobolev embedding. In turn, these terms can be controlled with the help of Young inequality, as in (5.35).

The terms involving $\check{e}^k$ can be handled by a standard Cauchy inequality, and a coefficient $\left\|\phi^{k+1}\right\|_\infty^2$ has to be included in the estimate (5.36). Such a bound is not available at present; it has to be obtained from a preliminary estimate before a discrete Gronwall inequality is applied; see the analysis in later subsections.

For the nonlinear expansion in (5.19), we make the nonlinear coefficient of order $O(s)$, as analyzed by (5.24) to (5.26). In addition, such a nonlinear coefficient has to be $\check{\Phi}$ dependent, instead of ϕ dependent, since we have not had the divided difference bound (in time) for the numerical solution. With such an $O(s)$ analysis, the nonlinear inner-product associated with (5.19) is bounded by (5.27), in which the first part can be controlled by the diffusion term and the second part is an $O(s^2)$ increment. The stability of such an $O(s^2)$ incremental term is ensured by the term $\left\|\nabla_h\check{e}^{k+1}\right\|_2^2-\left\|\nabla_h\check{e}^k\right\|_2^2$, which appears in (5.5) in Proposition 5.1, the estimate of the concave diffusion term.

Remark 5.4. For the 3D case, a discrete Sobolev embedding gives

$$\left\|\check{e}^{k+1/2}\right\|_4\le C\left\|\check{e}^{k+1/2}\right\|_2^{\frac{1}{4}}\cdot\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^{\frac{3}{4}},\quad\text{if }\left(\check{e}^{k+1/2}\middle\|\mathbf{1}\right)=0,\tag{5.45}$$

which is analogous to (5.32) in 2D; also see the related discussions in Guan et al.[48] In turn, we are able to derive the following result

$$\begin{aligned} &2h^3\left(\eta\left(\check{\Phi}^k,\check{\Phi}^{k+1}\right)-\eta\left(\phi^k,\phi^{k+1}\right)\left|\!\left|\!\left|\Delta_h\check{e}^{k+1/2}\right|\!\right|\!\right|\right)\\ &\le\frac{C_1}{\alpha^7}\left(\left\|\check{e}^k\right\|_2^2+\left\|\check{e}^{k+1}\right\|_2^2\right)+\alpha\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^2\\ &\quad+\frac{C_1}{\alpha}s^2\left\|\nabla_h\check{e}^k\right\|_2^2+\frac{C_1}{\alpha}\left(1+\left\|\phi^{k+1}\right\|_\infty^2\right)\left\|\check{e}^k\right\|_2^2,\quad\forall\alpha>0, \end{aligned}\tag{5.46}$$

the only changes being the α^7 replaces α^3 and we use the triple summation $(\cdot\,|||\,\cdot)$. As a result, a full order convergence in 3D can be derived in the same manner. The details are omitted in this paper for the sake of brevity.

5.3 | Proof of Theorem 2.12: $\ell^\infty(0,T;\ell^2)$ convergence

We begin with an $O(s^3+h^4)$ convergence assumption of the numerical solution, in ℓ^2 norm, up to time step t^k:

$$\left\|\check{e}^j\right\|_2\le C_{11}e^{C_{12}t^j}\left(s^3+h^4\right),\quad\forall 0\le j\le k,\tag{5.47}$$

with C_{11}, C_{12} independent on s and h. Consequently, an application of inverse inequality shows that

$$\left\|\check{e}^j\right\|_\infty+\left\|\nabla_h\check{e}^j\right\|_\infty\le\frac{C\|\check{e}^j\|_2}{h^{\frac{d}{2}+1}}\le\frac{CC_{11}e^{C_{12}t^j}\left(s^3+h^4\right)}{h^{\frac{d}{2}+1}}\le Ch^{1/2}\le 1,\quad\forall 0\le j\le k,\tag{5.48}$$

with the dimension $d=2$ or 3. It is also noted that the linear refinement constraint, $s\le Ch$, is used in the above derivation. In turn, the a priori assumption (5.13) for the numerical solution at t^k is valid by setting

$$C_0=\max_{0\le j\le k}\left(\left\|\check{\Phi}^j\right\|_\infty+\left\|\nabla_h\check{\Phi}^j\right\|_\infty\right)+1.\tag{5.49}$$

Moreover, it is clear that an estimate for $\left\|\phi^{k+1}\right\|_\infty$ is needed in the application of Proposition 5.2 in the nonlinear analysis. For this quantity, we observe that (5.12), which comes from a global in time ℓ^4 bound for the numerical solution (as derived in Theorem 2.10), implies that

$$\left\|\phi^{k+1}\right\|_\infty\le\frac{C\|\phi^{k+1}\|_4}{h^{\frac{d}{4}}}\le CC_0h^{-\frac{d}{4}},\quad\text{with } d \text{ the dimension},\tag{5.50}$$

in which the first step comes from a similar inverse inequality.

Now, we derive the ℓ^2 convergence at time step t^{k+1}. Multiplying by $2h^2\check{e}^{k+1/2}=h^2(\check{e}^{k+1}+\check{e}^k)$, summing over i and j, and applying Green's second identity (Proposition A.3), we have

$$\begin{aligned} &\left\|\check{e}^{k+1}\right\|_2^2-\left\|\check{e}^k\right\|_2^2+2B_cs\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^2\\ &=2h^2s\left(\eta\left(\check{\Phi}^k,\check{\Phi}^{k+1}\right)-\eta\left(\phi^k,\phi^{k+1}\right)|\!|\!|\Delta_h\check{e}^{k+1/2}\right)+2sh^2\left(\hat{\tau}^k|\!|\!|\check{e}^{k+1/2}\right)\\ &\quad-2B_esh^2\left(\hat{\check{e}}^{k+1/2}|\!|\!|\Delta_h\check{e}^{k+1/2}\right)-2h^2s\left(\left[J\star\hat{\check{e}}^{k+1/2}\right]|\!|\!|\Delta_h\check{e}^{k+1/2}\right). \end{aligned}\tag{5.51}$$

Applying Propositions 5.1 and 5.2 for linear and nonlinear errors, and using the Cauchy inequality to bound the truncation error term

$$2h^2s\left(\hat{\tau}^k\left\|\check{e}^{k+1/2}\right\|\right)\le sC_{13}\left(s^3+h^4\right)^2+s\left\|\check{e}^{k+1/2}\right\|_2^2\le sC_{13}\left(s^3+h^4\right)^2+\frac{s}{2}\left(\left\|\check{e}^{k+1}\right\|_2^2+\left\|\check{e}^k\right\|_2^2\right),\tag{5.52}$$

we arrive at

$$\begin{aligned} &\left\|\check{e}^{k+1}\right\|_2^2-\left\|\check{e}^k\right\|_2^2+s\left(2B_c-5B_e-2\alpha\right)\left\|\nabla_h\check{e}^{k+1/2}\right\|_2^2+B_es\left(\left\|\nabla_h\check{e}^{k+1}\right\|_2^2-\left\|\nabla_h\check{e}^k\right\|_2^2\right)\\ &\le\frac{C_1}{\alpha^3}s\left(\left\|\check{e}^k\right\|_2^2+\left\|\check{e}^{k+1}\right\|_2^2\right)+\frac{C_{14}}{\alpha}s\left(\left\|\check{e}^k\right\|_2^2+\left\|\check{e}^{k-1}\right\|_2^2\right)+B_es\left\|\nabla_h\check{e}^{k-1/2}\right\|_2^2\\ &\quad+\frac{C_1}{\alpha}s^3\left\|\nabla_h\check{e}^k\right\|_2^2+\frac{C_1}{\alpha}s\left\|\phi^{k+1}\right\|_\infty^2\left\|\check{e}^k\right\|_2^2+sC_{13}\left(s^3+h^4\right)^2,\quad\forall\alpha>0. \end{aligned}\tag{5.53}$$

5.3.1 | A preliminary estimate for $\left\|\phi^{k+1}\right\|_\infty$

Note that an $O(1)$ bound for $\left\|\phi^{k+1}\right\|_\infty$ is not available at this point, because of the lack of information of the numerical solution at time step t^{k+1}. We only have (5.50), which comes from an unconditional ℓ^4 stability of the numerical solution, and this bound may become singular as $h \to 0$. Meanwhile, such a bound is needed to apply the Gronwall inequality.

To overcome this difficulty, we derive an estimate, based on (5.53), the assumption (5.47) (up to time step t^k), and the preliminary bound (5.50). The assumption (5.47) implies that

$$\left\|\check{e}^k\right\|_2^2 \le Ch^6, \quad \left\|\nabla_h \check{e}^k\right\|_2^2, \left\|\nabla_h \check{e}^{k-1/2}\right\|_2^2 \le Ch^4, \quad \left\|\phi^{k+1}\right\|_\infty^2 \le Ch^{-\frac{d}{2}}, \tag{5.54}$$

with the standard constraint $s \le Ch$. Furthermore, using the fact that $\alpha_0 = B_c - 3B_e > 0$ and taking $\alpha = \frac{\alpha_0}{2}$, we conclude from (5.53) that

$$\left\|\check{e}^{k+1}\right\|_2^2 \le C\left(h^5 + h^{7-\frac{d}{2}}\right) \le Ch^5, \quad \text{since } 7 - \frac{d}{2} > 5 \text{ for } d = 2, 3. \tag{5.55}$$

In turn, an application of inverse inequality shows that

$$\left\|\check{e}^{k+1}\right\|_\infty \le \frac{C\|\check{e}^{k+1}\|_2}{h^{\frac{d}{2}}} \le Ch^{\frac{5}{2}-\frac{d}{2}} \le Ch \le 1, \quad \text{with } d = 2 \text{ or } 3. \tag{5.56}$$

Consequently, the triangular inequality yields

$$\left\|\phi^{k+1}\right\|_\infty \le \left\|\check{\Phi}^{k+1}\right\|_\infty + \left\|\check{e}^{k+1}\right\|_\infty \le C_{15} := C_0 + 1. \tag{5.57}$$

Remark 5.5. Of course, the rough estimate (5.55) is not the convergence result that we want. Not only its accuracy is not satisfactory, $O(h^{\frac{5}{2}})$ instead of $O(s^3 + h^4)$, but also its stability is not maintained: $O(s^3 + h^4)$ convergence at the previous time step to an order $O(h^{\frac{5}{2}})$ at the next time step. The reason for such an accuracy deterioration is due to the singular bound (5.50) for $\left\|\phi^{k+1}\right\|_\infty$, which comes from the global in time ℓ^4 bound for the numerical solution. The purpose of the rough estimate (5.55) is to derive a preliminary "convergence" result in the ℓ^2 norm, based on the full convergence result at the previous time step, combined with the singular bound (5.50), so that a regular $O(1)$ bound can be obtained for the $\|\cdot\|_\infty$ norm of the numerical solution at the next time step with an application of inverse inequality. Subsequently, the full order ℓ^2 convergence at the next time step can be derived by using the discrete Gronwall inequality, since an $O(1)$ bound for $\left\|\phi^{k+1}\right\|_\infty$ has been available.

5.3.2 | $\ell^\infty(0, T; \ell^2)$ convergence and a recovery of the assumption (5.47)

A substitution of (5.57) into (5.53) gives

$$\begin{aligned} &\left\|\check{e}^{k+1}\right\|_2^2 - \left\|\check{e}^k\right\|_2^2 + s\left(2B_c - 5B_e - 2\alpha\right)\left\|\nabla_h \check{e}^{k+1/2}\right\|_2^2 + B_e s\left(\left\|\nabla_h \check{e}^{k+1}\right\|_2^2 - \left\|\nabla_h \check{e}^k\right\|_2^2\right) \\ \le\ & \frac{C_{16}}{\alpha^3} s\left(\left\|\check{e}^k\right\|_2^2 + \left\|\check{e}^{k+1}\right\|_2^2\right) + \frac{C_{14}}{\alpha} s\left\|\check{e}^{k-1}\right\|_2^2 + B_e s\left\|\nabla_h \check{e}^{k-1/2}\right\|_2^2 \\ &+ \frac{C_1}{\alpha} s^3\left\|\nabla_h \check{e}^k\right\|_2^2 + sC_{13}\left(s^3 + h^4\right)^2, \quad \forall \alpha > 0. \end{aligned} \tag{5.58}$$

Replacing the index k by l, summing on l, from $l = 0$ to $l = k$, and using $\check{e}^0 \equiv 0$ (by (4.15)), we have

$$\begin{aligned} &\left\|\check{e}^{k+1}\right\|_2^2 + B_e s\left\|\nabla_h \check{e}^{k+1}\right\|_2^2 + s\left(2\alpha_0 - 2\alpha\right)\sum_{l=1}^k \left\|\nabla_h \check{e}^l\right\|_2^2 \\ \le\ & s\left(\frac{C_{16}}{\alpha^3} + \frac{C_{14}}{\alpha}\right)\sum_{l=1}^k \left\|\check{e}^l\right\|_2^2 + s\frac{C_{16}}{\alpha^3}\sum_{l=0}^k \left\|\check{e}^{l+1}\right\|_2^2 + \frac{C_1}{\alpha} s^3 \sum_{l=0}^k \left\|\nabla_h \check{e}^l\right\|_2^2 + sC_{13}\sum_{l=0}^k (h^4 + s^3)^2, \end{aligned} \tag{5.59}$$

with $B_c - 3B_e = \alpha_0 > 0$ as in (2.48). As a direct consequence, by taking $\alpha = \frac{\alpha_0}{2}$, the following inequality holds:

$$\frac{1}{1 - C_{17}s}\left\|\check{e}^{k+1}\right\|_2^2 + B_e s\left\|\nabla_h \check{e}^{k+1}\right\|_2^2 \le s\frac{C_{18}}{\alpha_0^3}\sum_{l=1}^k \left\|e^l\right\|_2^2 + \frac{C_1}{\alpha} s^3 \sum_{l=0}^k \left\|\nabla_h \check{e}^l\right\|_2^2 + sC_{13}\sum_{l=0}^k (h^4 + s^3)^2, \tag{5.60}$$

with $C_{17} := \frac{C_{16}}{\alpha^3}$ and $C_{18} := C_{16} + C_{14}\alpha^2$. We can always choose s with $1 - C_{17}s \geqslant \frac{1}{2}$. In turn, by denoting

$$G^l = 2\left\|\check{e}^l\right\|_2^2 + B_e s\left\|\nabla_h \check{e}^l\right\|_2^2, \tag{5.61}$$

we get

$$G^{k+1} \leq 2s\frac{C_{18}}{\alpha_0^3}\sum_{l=1}^{k} G^l + sC_{13}\sum_{l=0}^{k}(h^4 + s^3)^2, \tag{5.62}$$

with the choice of s so that $\frac{C_1 s}{\alpha} \leq 2B_e$. An application of the discrete Gronwall inequality yields the desired result:

$$\left\|\check{e}^{k+1}\right\|_2^2 \leq G^{k+1} \leq C_{19}\left(s^3 + h^4\right)^2, \quad \text{so that } \left\|\check{e}^{k+1}\right\|_2 \leq \sqrt{C_{19}}\left(s^3 + h^4\right), \tag{5.63}$$

with C_{19} independent on s and h. A more detailed exploration implies the structure of this constant: $C_{19} = C_{11}e^{C_{12}t^{k+1}}$. As a result, the a priori assumption (5.47) is recovered at the time step t^{k+1} so that an $O(s^4 + h^4)$ convergence in ℓ^2 norm, between the numerical solution and the constructed approximate solution $\check{\Phi}$, has been established, using an induction argument.

Finally, the proof of Theorem 2.12 can be completed with the following application of triangle inequality:

$$\left\|e^l\right\|_2 = \left\|\phi^l - \Phi^l\right\|_2 \leq \left\|\phi^l - \check{\Phi}^l\right\|_2 + \left\|\Phi^l - \check{\Phi}^l\right\|_2 \leq C\left(s^2 + h^2\right), \quad \forall l \cdot s \leq T, \tag{5.64}$$

in which the error estimate (5.63) and the analysis (5.1) for the constructed solution are used.

Remark 5.6. The assumption (2.48) (for the physical parameters) is required in the convergence analysis for the nCH equation. Such an assumption is necessary for the convex diffusion part to control the concave diffusion part, because of a subtle estimate (5.5). As a consequence of this inequality, the assumption $B_c > 3B_e$ has to be made to make the convergence analysis pass through. In comparison, for the nAC equation, this assumption is not required, as explained in Remark 3.2.

On the other hand, our extensive numerical experiments have implied that such an assumption only corresponds to a technical difficulty in the convergence analysis. For most practical computational models, the second-order convergence is well preserved as long as the positive-diffusivity condition (2.5) is valid.

Remark 5.7. We note that the second-order $\ell^\infty(0, T; \ell^2)$ convergence for the nCH equation is conditional, ie, under a mild linear refinement constraint, $s \leq Ch$. In comparison, the $\ell^\infty(0, T; \ell^2)$ convergence for the nAC equation is unconditional, as explained in Remark 3.1.

Such a subtle difference comes from the analysis techniques for the nonlinear inner-products. For the nAC equation, the decomposition (3.10) has greatly facilitated the error estimates, and the maximum norm bound of the numerical solution is not needed in the derivation. However, for the nCH equation, since the discrete H^1 inner-product of $\check{e}^{k+1/2}$ and the nonlinear error function have to be analyzed, we need to make an a priori assumption (5.47) at the previous time step, obtain a discrete $W^{1,\infty}$ bound of the numerical solution, and the $\ell^\infty(0, T; \ell^2)$ convergence estimate justifies the a priori assumption at the next time step. This process is further facilitated by the higher order consistency analysis presented in Section 4.

5.4 | Proof of Theorem 2.13: $\ell^\infty(0, T; \ell^\infty)$ convergence

With the $O(s^3 + h^4)$ convergence result (5.63), in ℓ^2 norm, we apply the inverse inequality and get

$$\left\|\check{e}^{k+1}\right\|_\infty \leq \frac{C\left\|\check{e}^{k+1}\right\|_2}{h^{\frac{d}{2}}} \leq \frac{C\sqrt{C_{19}}\left(s^3 + h^4\right)}{h^{\frac{d}{2}}} \leq C_{20}\left(s^2 + h^2\right), \quad \text{with } d = 2, \tag{5.65}$$

with the linear refinement constraint $s \leq Ch$ and $C_{20} = C\sqrt{C_{19}}$. For the 3D case, a higher order asymptotic expansion of the numerical solution has to be performed so that an $O(s^4 + h^4)$ consistency and convergence in ℓ^2 norm are obtained. The details are left to interested readers.

Subsequently, by combining the ℓ^∞ error estimate (5.65) and the analysis (5.1) for the constructed solution, we finish the proof of Theorem 2.12 with an application of triangle inequality:

$$\left\|e^l\right\|_\infty = \left\|\phi^l - \Phi^l\right\|_\infty \leq \left\|\phi^l - \check{\Phi}^l\right\|_\infty + \left\|\Phi^l - \check{\Phi}^l\right\|_\infty \leq C\left(s^2 + h^2\right), \quad \forall l \cdot s \leq T. \tag{5.66}$$

Remark 5.8. In fact, in the a priori assumption (5.47), the detailed form of constants C_{11} and C_{12} has not been fixed; instead, these 2 constants are fixed by inequality (5.63), with $C_{19} = C_{11}e^{C_{12}t^{k+1}}$. In more details, C_{11} and C_{12} depend on the constants $C_{13}, C_{14}, \ldots, C_{18}$.

However, this argument does not cause the trouble of a cycling analysis, because of the subtle fact that the subsequent constants $C_{13}, \ldots, C_{18}$ do not depend on C_{11} and C_{12}. In fact, for the a priori assumption (5.47), we only require that C_{11} and C_{12} are bounded by a fixed constant, so that inequality (5.48) becomes valid. With the availability of (5.48), all the subsequent constants $C_{13}, \ldots, C_{18}$ do not depend on C_{11} and C_{12} at all.

5.5 | The $\ell^\infty(0,T;\ell^\infty)$ convergence for the nAC equation

For the second-order convex splitting scheme (2.30) for the nAC equation, the higher order consistency analysis could be performed in the same manner as in Section 4. In turn, an $\ell^\infty(0,T;\ell^2)$ convergence estimate with an improved order $O(s^3+h^4)$ is expected, and an application of inverse inequality leads to a similar $\ell^\infty(0,T;\ell^\infty)$ convergence result as Theorem 2.13, under the linear refinement path constraint $s \le Ch$. The proof of the following theorem is skipped for brevity, and the details are left to interested readers.

Theorem 5.9. *Under the assumptions of Theorem 2.11, we also have optimal order convergence of the numerical solution of the scheme (2.30) in the ℓ^∞ norm. Namely, if s and h are sufficiently small with the linear refinement path constraint $s \le Ch$, with C any fixed constant, we have*

$$\left\| e^l \right\|_\infty \le C\left(h^2 + s^2\right), \tag{5.67}$$

where $C > 0$ is independent of h and s.

6 | NUMERICAL RESULTS

In this section, we present a few numerical experiments, verifying the convergence results of the second-order schemes for the nCH and nAC equations.

6.1 | Numerical convergence for the nCH equation

Here we discuss the numerical results for the nCH equation. We present 2 cases, based on the restriction proposed in Equation 2.48. These experiments verify the convergence rate in the $\ell^\infty(0,T;\ell^2)$ norm. We use a square domain $\Omega = (-0.5, 0.5)^2$ with smooth, periodic initial data $0.5\sin(2\pi x_1)\sin(2\pi x_2)$. The convolution kernel J is taken to be

$$\mathsf{J} = \alpha \exp\left(-\frac{x_1^2 + x_2^2}{\sigma^2}\right), \tag{6.1}$$

where $\sigma = 0.05$ and $\alpha = \frac{1}{\sigma^2}$. We extend J periodically outside of Ω. The other parameters are $\gamma_c = 4$ and $\gamma_e = 0$ in the first case, which yield $\alpha_0 = 4 - \pi > 0$; and $\gamma_c = 0$ and $\gamma_e = 1$ in the second case, which yield $\alpha_0 = -3 - \pi < 0$. The final time for the tests is given by $T = 0.01$. To verify the spatial convergence order, we fix $s = 10^{-4}$ and compare the difference function e_A with respect to $h = 1/64, 1/128, 1/256, 1/512$, and $1/1024$. Since we do not have the exact solution—these are not easily obtained for nontrivial convolution kernels—we are using the difference between results on successive coarse and fine grids for the numerical comparison. The difference function, e_A, is evaluated at time $T = 0.01$ using the method described in previous studies.[48,58,59] To verify the temporal convergence order, we fix $h = 1/1024$ and compare the difference function e_A with respect to $s = 0.001, 0.0005, 0.00025, 0.000125, 0.0000625$, and 0.00003125. The result is displayed in Tables 1 and 2 ($\alpha_0 = 4-\pi > 0$) and Tables 3 and 4 ($\alpha_0 = -3-\pi < 0$) . In both cases, the spatial and temporal second-order accuracy of the method is confirmed.

6.2 | Numerical convergence for the nAC equation

Here we discuss the numerical results for the nAC equation. First we present the experiment verifying the numerical convergence rate. The setting of the experiment is the same as the nCH case, with $\gamma_c = 0$ and $\gamma_e = 1$ which yields $\alpha_0 = -3 - \pi < 0$. The result is displayed in Tables 5 and 6. The spatial and temporal second-order accuracy of the method is confirmed.

TABLE 1 The difference between coarse and fine spatial discretization of the computed numerical solutions, with $\alpha_0 = 4 - \pi$ and $s = 0.0001$

Coarse h	Fine h	$\|e_A\|_2$	Rate
1/64	1/128	2.391350720781724e-05	—
1/128	1/256	5.973631155837239e-06	2.001145668661347
1/256	1/512	1.493114545413543e-06	2.000283313475169
1/512	1/1024	3.732652648708757e-07	2.000051680742358

The second-order spatial convergence of the method is confirmed in the test.

TABLE 2 The difference between coarse and fine temporal discretization of the computed numerical solutions, with $\alpha_0 = 4 - \pi$ and $h = 1/1024$

Coarse s	Fine s	$\|e_A\|_2$	Rate
0.001	0.0005	0.001794295721092	—
0.0005	0.00025	0.000398264862447	2.171617576649190
0.00025	0.000125	0.000095965882587	2.053134700418730
0.000125	0.0000625	0.000023646151477	2.020916198465040

The second-order temporal convergence of the method is confirmed in the test.

TABLE 3 The difference between coarse and fine spatial discretization of the computed numerical solutions, with $\alpha_0 = -3 - \pi$ and $s = 0.0001$

Coarse h	Fine h	$\|e_A\|_2$	Rate
1/64	1/128	1.889677031506123e-04	—
1/128	1/256	4.731605521752042e-05	1.997737976601742
1/256	1/512	1.183367120319446e-05	1.999432084207052
1/512	1/1024	2.958708490313346e-06	1.999858250001422

The second-order spatial convergence of the method is confirmed in the test.

TABLE 4 The difference between coarse and fine temporal discretization of the computed numerical solutions, with $\alpha_0 = -3 - \pi$ and $h = 1/1024$

Coarse s	Fine s	$\|e_A\|_2$	Rate
0.001	0.0005	0.014086218352630	—
0.0005	0.00025	0.003381770927788	2.058433507623583
0.00025	0.000125	0.000818756993775	2.046271708593699
0.000125	0.0000625	0.000202980831200	2.012091834242648

The second-order temporal convergence of the method is confirmed in the test.

TABLE 5 The difference between coarse and fine spatial discretization of the computed numerical solutions, with $\gamma_0 = -3 - \pi$ and $s = 0.0001$

Coarse h	Fine h	$\|e_A\|_2$	Rate
1/128	1/256	1.516375102958663e-04	–
1/256	1/512	3.791508908862791e-05	1.999782656594734
1/512	1/1024	9.479128597637906e-06	1.999945767307481
1/1024	1/2048	2.369804223848923e-06	1.999986561407764

The second-order spatial convergence of the method is confirmed in the test.

We also present experiments of phase separation described by the nAC equation under the following conditions: **1)**$\Omega = (-10, 10)^2$; **2)** the size of time step is $s = 0.01$, the number of nodes on grid is 512^2 and the total number of time iterations is

TABLE 6 The difference between coarse and fine temporal discretization of the computed numerical solutions, with $\alpha_0 = -3 - \pi$ and $h = 1/1024$

Coarse s	Fine s	$\|e_A\|_2$	Rate
0.001	0.0005	4.793803762722221e-07	—
0.0005	0.00025	1.198778499378929e-07	1.999605738770943
0.00025	0.000125	2.997276971768256e-08	1.999840802426613
0.000125	0.0000625	7.494493907180996e-09	1.999749442912903

The second-order temporal convergence of the method is confirmed in the test.

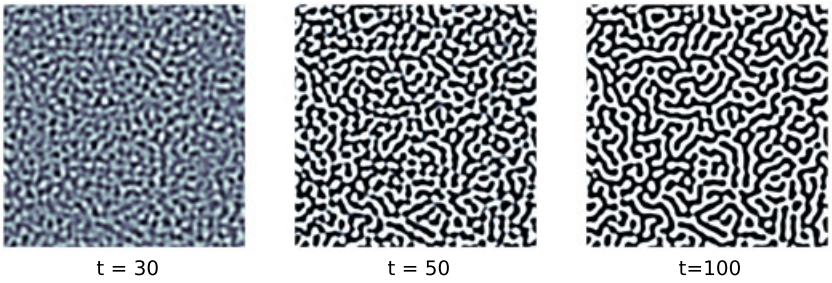

FIGURE 1 Phase separation described by nonlocal Allen-Cahn equation [Colour figure can be viewed at wileyonlinelibrary.com]

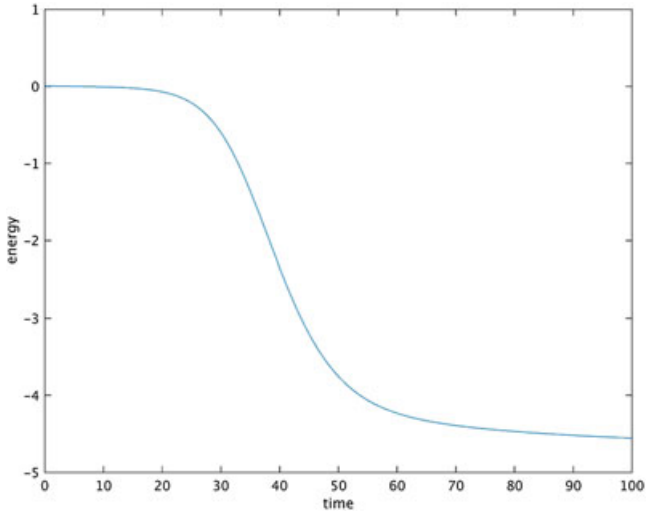

FIGURE 2 Energy evolution of phase separation [Colour figure can be viewed at wileyonlinelibrary.com]

10^4; **3)** The convolution kernel J is a function defined as the difference between 2 Gaussians:

$$\mathsf{J} = \alpha \exp\left(-\frac{x_1^2 + x_2^2}{\sigma_1^2}\right) - \beta \exp\left(-\frac{x_1^2 + x_2^2}{\sigma_2^2}\right), \tag{6.2}$$

where $\sigma_1 = 0.16$, $\sigma_2 = 0.4$, $\alpha = \frac{0.1}{\sigma_1^2}$ and $\beta = \frac{0.08}{\sigma_2^2}$; **4)**$\gamma_e = 0$, $\gamma_c = 0$. The initial condition of the simulation is a random perturbation of the constant state $\phi_{ave} = 0$. Figure 1 shows snapshots of the evolution up to time T = 100, and Figure 2 shows the corresponding numerical energy for the simulation. The energy is observed to decay as time increases.

7 | CONCLUDING REMARKS

In this paper, we have presented the detailed convergence analyses for fully discrete second-order numerical schemes for nAC and nCH equations. For the nAC equation, the standard procedure of consistency and stability estimates indicates the desired convergence result, without any constraint between time step s and spatial grid size h, in which a careful nonlinear expansion

has been used. For the nCH equation, such an approach does not work directly, and we have to an H^{-1} inner-product estimate of this nonlinear numerical error is derived to establish convergence. In addition, because of the complicated form of the nonlinear term, a careful expansion of its discrete gradient is necessary. In the convergence analysis for the nCH equation, an a priori $W^{1,\infty}$ bound of the numerical solution at the discrete level has to be set, to pass through the error estimate. Such a bound can be obtained by performing a higher order consistency analysis, up to accuracy order $O(s^3 + h^4)$, by using asymptotic expansions for the numerical solution. In turn, instead of a direct comparison between the exact and numerical solutions, an error estimate between the numerical solution and the constructed approximate solution yields a higher order convergence in $\ell^\infty(0, T; \ell^2)$ norm, and such a result yields the necessary bound under a standard constraint $s \le Ch$. Moreover, the convergence in the ℓ^∞ norm is also proved in this paper, under the same constraint.

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APPENDIX A: FINITE DIFFERENCE DISCRETIZATION OF SPACE

Our primary goal in this appendix is to define some finite-difference operators and provide some summation-by-parts formulas in 1 and 2 space dimensions that are used to derive and analyze the numerical schemes. Everything extends straightforwardly to 3D. We make extensive use of the notation and results for cell-centered functions from two studies.[57,58] The reader is directed to those references for more complete details.

In 1D we will work on the interval $\Omega = (0, L)$, with $L = m \cdot h$, and in 2D, we work with the rectangle $\Omega = (0, L_1) \times (0, L_2)$, with $L_1 = m \cdot h$ and $L_2 = n \cdot h$, where m and n are positive integers and $h > 0$ is the spatial step size. Define $p_r := (r - \frac{1}{2}) \cdot h$, where r takes on integer or half-integer values. For any positive integer ℓ, define $E_\ell = \left\{ p_r \mid r = \frac{1}{2}, \ldots, \ell + \frac{1}{2} \right\}$, $C_\ell = \{ p_r \mid r = 1, \ldots, \ell \}$, $C_{\bar{\ell}} = \{ p_r \cdot h \mid r = 0, \ldots, \ell + 1 \}$. We need the 1D grid function spaces

$$\mathcal{C}_m = \{ \phi : C_m \to \mathbb{R} \}, \ \mathcal{E}_m = \{ u : E_m \to \mathbb{R} \},$$

and the 2D grid function spaces

$$\mathcal{C}_{m\times n} = \{ \phi : C_m \times C_n \to \mathbb{R} \}, \qquad \mathcal{V}_{m\times n} = \{ f : E_m \times E_n \to \mathbb{R} \},$$
$$\mathcal{E}^{\text{ew}}_{m\times n} = \{ u : E_m \times C_n \to \mathbb{R} \}, \qquad \mathcal{E}^{\text{ns}}_{m\times n} = \{ v : C_m \times E_n \to \mathbb{R} \}.$$

We use the notation $\phi_{i,j} := \phi\left(p_i, p_j\right)$ for *cell-centered* functions, ie, those in the space $\mathcal{C}_{m\times n}$. In component form *east-west edge-centered* functions, ie, those in the space $\mathcal{E}^{\text{ew}}_{m\times n}$, are identified via $u_{i+\frac{1}{2},j} := u(p_{i+\frac{1}{2}}, p_j)$. In component form *north-south edge-centered* functions, ie, those in the space $\mathcal{E}^{\text{ns}}_{m\times n}$, are identified via $u_{i+\frac{1}{2},j} := u(p_{i+\frac{1}{2}}, p_j)$. The functions of $\mathcal{V}_{m\times n}$ are called *vertex-centered* functions. In component form vertex-centered functions are identified via $f_{i+\frac{1}{2},j+\frac{1}{2}} := f(p_{i+\frac{1}{2}}, p_{j+\frac{1}{2}})$. The 1D cell-centered and edge-centered functions are easier to express.

We will need the weighted 2D discrete inner-products $(\cdot \| \cdot)$, $[\cdot \| \cdot]_{\text{ew}}$, $[\cdot \| \cdot]_{\text{ns}}$ that are defined in two studies[57,58]:

$$(\phi \| \psi) = \sum_{i=1}^{m} \sum_{j=1}^{n} \phi_{i,j} \psi_{i,j}, \ \phi, \psi \in \mathcal{C}_{m\times n}, \tag{A1}$$

$$\left[f \| g \right]_{\text{ew}} = \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{n} \left(f_{i+\frac{1}{2},j} g_{i+\frac{1}{2},j} + f_{i-\frac{1}{2},j} g_{i-\frac{1}{2},j} \right), \ f, g \in \mathcal{E}^{\text{ew}}_{m\times n}, \tag{A2}$$

$$\left[f \| g \right]_{\text{ns}} = \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{n} \left(f_{i,j+\frac{1}{2}} g_{i,j+\frac{1}{2}} + f_{i,j-\frac{1}{2}} g_{i,j-\frac{1}{2}} \right), \ f, g \in \mathcal{E}^{\text{ns}}_{m\times n}. \tag{A3}$$

In addition to these, we will use the 2D discrete inner-product

$$\begin{aligned} \langle f \| g \rangle = \frac{1}{4} \sum_{i=1}^{m} \sum_{j=1}^{n} \big(& f_{i+\frac{1}{2},j+\frac{1}{2}} g_{i+\frac{1}{2},j+\frac{1}{2}} + f_{i+\frac{1}{2},j-\frac{1}{2}} g_{i+\frac{1}{2},j-\frac{1}{2}} \\ & + f_{i-\frac{1}{2},j+\frac{1}{2}} g_{i-\frac{1}{2},j+\frac{1}{2}} + f_{i-\frac{1}{2},j-\frac{1}{2}} g_{i-\frac{1}{2},j-\frac{1}{2}} \big), \quad f, \ g \in \mathcal{V}^{\text{ns}}_{m\times n}. \end{aligned} \tag{A4}$$

We shall say the cell-centered function $\phi \in \mathcal{C}_{m\times n}$ is periodic if and only if, for all $p,\ q \in \mathbb{Z}$,

$$\phi_{i+p\cdot m,j+q\cdot n} = \phi_{i,j} \quad i = 1, \ldots, m, \quad j = 1, \ldots, n. \tag{A5}$$

Here we have abused notation a bit, since ϕ is not explicitly defined on an infinite grid. Of course, ϕ can be extended as a periodic function in a perfectly natural way, which is the context in which we view the last definition. Similar definitions are implied for periodic edge-centered and vertex-centered grid functions. The 1D and 3D cases are analogous and are suppressed.

The reader is referred to previous studies[57,58] for the precise definitions of the edge-to-center difference operators $d_x : \mathcal{E}^{\text{ew}}_{m\times n} \to \mathcal{C}_{m\times n}$ and $d_y : \mathcal{E}^{\text{ns}}_{m\times n} \to \mathcal{C}_{m\times n}$; the x-dimension center-to-edge average and difference operators, respectively, $A_x,\ D_x : \mathcal{C}_{m\times n} \to \mathcal{E}^{\text{ew}}_{m\times n}$; the y-dimension center-to-edge average and difference operators, respectively, $A_y,\ D_y : \mathcal{C}_{m\times n} \to \mathcal{E}^{\text{ns}}_{m\times n}$; and the standard 2D discrete Laplacian, $\Delta_h : \mathcal{C}_{m\times n} \to \mathcal{C}_{m\times n}$. These operators have analogs in 1D and 3D that should be clear to the reader.

We will use the grid function norms defined in previous studies.[57,58] The reader is referred to those references for the precise definitions of $\|\cdot\|_2$, $\|\cdot\|_\infty$, $\|\cdot\|_p$ $(1 \le p < \infty)$, $\|\cdot\|_{0,2}$, $\|\cdot\|_{1,2}$, and $\|\phi\|_{2,2}$. We will specifically use the following inverse inequality in 2D: for any $\phi \in \mathcal{C}_{m\times n}$ and all $1 \le p < \infty$

$$\|\phi\|_\infty \le h^{-\frac{2}{p}} \|\phi\|_p. \tag{A6}$$

Again, the analogous norms in 1D and 3D should be clear.

Using the definitions given in this appendix and in previous studies,[57,58] we obtain the following summation-by-parts formulas whose proofs are simple:

Proposition A.1. *If $\phi \in \mathcal{C}_{m\times n}$ and $f \in \mathcal{E}^{ew}_{m\times n}$ are periodic then*

$$h^2 \left[D_x\phi \| f\right]_{ew} = -h^2 \ (\phi \| d_x f), \tag{A7}$$

and if $\phi \in \mathcal{C}_{m\times n}$ and $f \in \mathcal{E}^{ns}_{m\times n}$ are periodic then

$$h^2 \left[D_y\phi \| f\right]_{ns} = -h^2 \ \left(\phi \| d_y f\right). \tag{A8}$$

Proposition A.2. *Let $\phi,\ \psi \in \mathcal{C}_{\bar{m}\times\bar{n}}$ be periodic grid functions. Then*

$$h^2 \ [D_x\phi \| D_x\psi]_{ew} + h^2 \ \left[D_y\phi \| D_y\psi\right]_{ns} = -h^2 \ (\phi \| \Delta_h\psi). \tag{A9}$$

Proposition A.3. *Let $\phi,\ \psi \in \mathcal{C}_{m\times n}$ be periodic grid functions. Then*

$$h^2 \ (\phi \| \Delta_h\psi) = h^2 \ (\Delta_h\phi \| \psi). \tag{A10}$$

Analogs in 1D and 3D of the summation-by-parts formulas above are straightforward.