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A reaction-diffusion system of λ–ω type Part II: Numerical analysis

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We undertake the numerical analysis of a reaction-diffusion system of 'λ–ω' type [26]. Results are presented for a fully-practical piecewise linear finite element method by mimicking results in the continuous case [11]. We establish *a priori* estimates and error bounds for a semi-discrete and a fully discrete finite element approximation. The theoretical results are illustrated and verified via the numerical solution of periodic plane waves in one space dimension. Experiments in two space dimensions led to 'target patterns' and spiral wave break-up.

1 Introduction

Let $\Omega \subset \mathbb{R}^d$, $d \leqslant 3$, be an open, bounded, convex domain, and $\Omega_T := \Omega \times (0, T)$, $T > 0$. We study the approximate solutions of the following reaction-diffusion system of 'λ-ω' type [26]. Find $\{u(\mathbf{x}, t), v(\mathbf{x}, t)\}$ such that

$$\frac{\partial u}{\partial t} = \Delta u + \lambda(r)\, u - \omega(r)\, v \qquad \text{in} \quad \Omega_T, \tag{1.1a}$$

$$\frac{\partial v}{\partial t} = \Delta v + \omega(r)\, u + \lambda(r)\, v \qquad \text{in} \quad \Omega_T, \tag{1.1b}$$

$$u(\mathbf{x}, 0) = u_0(\mathbf{x}), \qquad v(\mathbf{x}, 0) = v_0(\mathbf{x}) \quad \mathbf{x} \in \Omega, \tag{1.1c}$$

$$\frac{\partial u}{\partial \boldsymbol{\nu}} = \frac{\partial v}{\partial \boldsymbol{\nu}} = 0 \quad \text{on} \quad \Sigma := \partial\Omega \times (0, T), \tag{1.1d}$$

where $\boldsymbol{\nu}$ denotes the outward normal to $\partial\Omega$ and the 'amplitude' is given by $r := \sqrt{u^2 + v^2}$. As in Blowey & Garvie [11], we take the λ and ω functions to be

$$\lambda(r) := \lambda_0 - \lambda_1 r^\rho, \qquad \omega(r) := \omega_0 + \omega_1 r^\rho, \tag{1.1e}$$

with real, finite parameters λ_0, λ_1, $\rho > 0$ and ω_0, $\omega_1 \neq 0$.

In the case $\rho = 2$, these equations are close to a supercritical Hopf bifurcation in the reaction kinetics and are model equations for oscillatory reaction-diffusion equations. The typical 'periodic plane wave' solutions are periodic (in space and time) travelling waves. In two space dimensions there is also the possibility of spiral waves, concentric ring waves

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('target patterns') and 'turbulence'. For additional details concerning the background to this problem see Blowey & Garvie [11] and the references therein.

We consider a more general class of nonlinear $\lambda(\cdot)$ and $\omega(\cdot)$ functions than was originally proposed in Kopell & Howard [26], with an arbitrary power of ρ instead of a quadratic power. This led to significant challenges in both the mathematical and numerical analysis of this problem, which forced us to make assumptions on the parameter ρ, due to technical results in this paper and in Blowey & Garvie [11]. To prove existence and uniqueness of the semi-discrete approximations, we require the following restrictions on the parameter ρ :

(A1) ρ is any finite, positive number if $d = 1, 2$ and

$$\rho \leqslant 4 \text{ if } d = 3,$$

and for strong solution results of the $\lambda - \omega$ system we assume (see [11]):

(A2)
$$\rho \in \begin{cases} (0, 4] & \text{if } d = 1, \\ (0, 2] & \text{if } d = 2, \\ (0, \frac{4}{3}] & \text{if } d = 3. \end{cases}$$

To prove error estimates we require an additional restriction on ρ, namely:

(A3)
$$\rho \in \begin{cases} [\frac{7}{6}, 4] & \text{if } d = 1, \\ [\frac{7}{6}, 2] & \text{if } d = 2, \\ [\frac{7}{6}, \frac{4}{3}] & \text{if } d = 3. \end{cases}$$

Using the Faedo-Galerkin method of Lions [30] and compactness arguments, Blowey & Garvie [11] proved the well-posedness of the strong solutions to the λ–ω system with a domain of class C^2. However, for numerical analysis we require a polygonal or polyhedral domain. Thus for ease of exposition in this paper we assume that the results in Blowey & Garvie [11] also hold in the polygonal/polyhedral setting, i.e. we assume the following result throughout:

Theorem 1.1 *Assume $\Omega \subset \mathbb{R}^d$, $d \leqslant 3$, is an open, bounded, convex domain, which is polygonal if $d = 2$ and polyhedral if $d = 3$. Let* (A2) *hold and assume that $u_0, v_0 \in H^1(\Omega)$, then there exists a unique strong solution $\{u, v\}$ to the $\lambda - \omega$ system* (1.1*a*)–(1.1*e*) *s.t.*

$$u, v \in L^2(0, T; H^2(\Omega)) \cap C([0, T]; H^1(\Omega)),$$
$$\frac{\partial u}{\partial t}, \frac{\partial v}{\partial t} \in L^2(\Omega_T).$$

Since Kopell & Howard [26] introduced the λ-ω system, to our knowledge there have been only two numerical studies of these systems, namely, a short paper comparing two numerical methods for a specific example in one space dimension [39], and a paper studying the numerical analysis of a related λ-ω system using a finite difference approach with a nonlinear multigrid method in two space dimensions [12]. Our approach to the numerical analysis of the λ-ω system uses the standard piecewise-linear finite element method with quadrature, which leads to 'mass lumping'. For papers that use this approach, or employ similar arguments and tools to our own [2, 6, 9, 10, 16, 18, 19, 32, 34, 35]

The paper is organised in the following way. In § 2 we review some tools needed for the subsequent analysis and cover the basic notation. In § 3 we use the finite element method with piecewise-linear basis functions to obtain a semi-discrete approximation, *a priori* bounds of the semi-discrete solutions and then a semi-discrete error bound. In § 4 these calculations provide the basis for obtaining a semi-implicit, fully discrete approximation, *a priori* bounds for various norms of the fully discrete solutions and the derivation of fully discrete error estimates. Finally, in § 5 some numerical experiments are performed in one and two space dimension and the fully discrete error bound is verified numerically in one space dimension. Our methodology relies on the continuous estimates presented in Blowey & Garvie [11].

2 Mathematical preliminaries

The λ-ω system rewritten in vector form is:

$$\mathbf{u}_t = \Delta\mathbf{u} + B\mathbf{u} + |\mathbf{u}|^\rho A\mathbf{u}, \quad \text{in} \quad \Omega_T, \tag{2.1a}$$

$$\mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x}), \quad \frac{\partial\mathbf{u}}{\partial\boldsymbol{\nu}} = \mathbf{0} \quad \text{on} \quad \Sigma, \tag{2.1b}$$

$$\text{where} \quad B = \begin{bmatrix} \lambda_0 & -\omega_0 \\ \omega_0 & \lambda_0 \end{bmatrix}, \ A = \begin{bmatrix} -\lambda_1 & -\omega_1 \\ \omega_1 & -\lambda_1 \end{bmatrix}, \ \mathbf{u} = \begin{bmatrix} u \\ v \end{bmatrix}. \tag{2.1c}$$

We note for later use the following identities, which hold for all $\mathbf{x} \in \mathbb{R}^2$:

$$(B\mathbf{x})\cdot\mathbf{x} = \lambda_0|\mathbf{x}|^2, \qquad (A\mathbf{x})\cdot\mathbf{x} = -\lambda_1|\mathbf{x}|^2, \tag{2.2a}$$

$$|B\mathbf{x}| = \sqrt{\lambda_0^2 + \omega_0^2}\,|\mathbf{x}|, \qquad |A\mathbf{x}| = \sqrt{\lambda_1^2 + \omega_1^2}\,|\mathbf{x}|. \tag{2.2b}$$

It will also be convenient to express the λ-ω system in the equivalent complex form:

$$c_t = \Delta c + [\lambda(|c|) + i\,\omega(|c|)]c \quad \text{in} \quad \Omega_T, \tag{2.3a}$$

$$c(x,0) = c_0(x), \quad \frac{\partial c}{\partial\boldsymbol{\nu}} = 0 \quad \text{on} \quad \Sigma, \tag{2.3b}$$

$$\text{where} \quad c := u + i\,v, \quad r := |c| \equiv \sqrt{u^2 + v^2}. \tag{2.3c}$$

The λ-ω systems (2.1*a*)–(2.1*c*) and (2.3*a*)–(2.3*c*) lead to the introduction of the following two (equivalent) weak formulations:

(P$_1$) Find $\mathbf{u}(\cdot,t) \in \{H^1(\Omega)\}^2$ such that $\mathbf{u}(\cdot,0) = \mathbf{u}_0(\cdot)$ and for almost every $t \in (0,T)$

$$\langle\mathbf{u}_t,\boldsymbol{\eta}\rangle + (\nabla\mathbf{u},\nabla\boldsymbol{\eta}) = (B\mathbf{u},\boldsymbol{\eta}) + (|\mathbf{u}|^\rho A\mathbf{u},\boldsymbol{\eta}) \qquad \forall\,\boldsymbol{\eta} \in \{H^1(\Omega)\}^2. \tag{2.4}$$

(P$_2$) Find $c(\cdot,0) \in \mathbb{H}^1(\Omega)$ such that $c_0(\cdot) := u_0(\cdot) + iv_0(\cdot)$ and for almost every $t \in (0,T)$

$$\langle c_t,\eta\rangle + (\nabla c,\nabla\eta) = (\lambda(|c|)c,\eta) + i(\omega(|c|)c,\eta) \qquad \forall\eta \in \mathbb{H}^1(\Omega), \tag{2.5}$$

where $\mathbb{H}^1(\Omega)$ is the 'complexified' space of $H^1(\Omega)$, i.e., if $u = u_1 + iu_2 \in \mathbb{H}^1(\Omega)$ then $u_j \in H^1(\Omega)$, $j = 1, 2$. A finite-dimensional version of (P$_2$) will help to prove the existence of the semi-discrete approximations, while a finite-dimensional version of (P$_1$) will lead to *a priori* estimates, uniqueness and a fully discrete approximation. We employ standard notation for the Sobolev spaces $W^{m,p}(\Omega)$, $m \in \mathbb{N}$, $p \in [1, \infty]$, with associated norms and semi-norms $\|\cdot\|_{m,p}$ and $|\cdot|_{m,p}$ respectively. $W^{m,2}(\Omega)$ is denoted $H^m(\Omega)$ with norm $\|\cdot\|_m$ and semi-norm $|\cdot|_m$ and additionally $W^{0,2}(\Omega) \equiv L^2(\Omega)$. The usual $L^2(\Omega)$ inner product over Ω with norm $\|\cdot\|_0$ is denoted $(\cdot,\cdot)$, except in the weak formulation (P$_2$) (and the associated finite-dimensional weak formulation – see § 3) where it is understood that $(z, w) := \int_\Omega z(x)\overline{w(x)}\,dx$. We also denote $\langle \cdot, \cdot \rangle$ to be the duality pairing between $(H^1(\Omega))'$ and $H^1(\Omega)$. For further details on the Banach/Sobolev spaces and spaces depending on time and space, see Temam [40] or Robinson [37]. We denote '$\overset{c}{\hookrightarrow}$' and '$\hookrightarrow$' to mean compact injection and continuous injection respectively. We also employ standard multi-index notation D^α for the mixed partial derivative of order $|\alpha|$ ($\alpha_i \in \mathbb{N} \cup \{0\}$).

Two key inequalities (cf. Blowey & Garvie [11]) are that the nonlinearity in (2.1a) is locally Lipschitz, namely, for all $\mathbf{u}_1, \mathbf{u}_2 \in \mathbb{R}^2$

$$||\mathbf{u}_1|^\rho A\mathbf{u}_1 - |\mathbf{u}_2|^\rho A\mathbf{u}_2| \leqslant (\rho + 1)\sqrt{\lambda_1^2 + \omega_1^2}\,(|\mathbf{u}_1|^\rho + |\mathbf{u}_2|^\rho)|\mathbf{u}_1 - \mathbf{u}_2|, \tag{2.6}$$

and we have the following monotonicity property: let $\mathbf{v}_1, \mathbf{v}_2 \in \mathbb{R}^n$, $n \in \mathbb{N}$, $p \geqslant 0$, then

$$|\mathbf{v}_1|^p \mathbf{v}_1 \cdot (\mathbf{v}_1 - \mathbf{v}_2) \geqslant \frac{|\mathbf{v}_1|^{p+2} - |\mathbf{v}_2|^{p+2}}{p+2}. \tag{2.7}$$

For later purposes we recall a Gagliardo–Nirenberg inequality, which is a Sobolev interpolation result (e.g. see Adams & Fournier [1]): let $s \in [1, \infty]$, $m \geqslant 1$ and assume $v \in W^{m,s}(\Omega)$. Then there are constants C and $\mu = \frac{d}{m}\left(\frac{1}{s} - \frac{1}{r}\right)$ such that the inequality

$$\|v\|_{0,r} \leqslant C\|v\|_{0,s}^{1-\mu}\|v\|_{m,s}^{\mu} \quad \text{holds for} \quad r \in \begin{cases} [s, \infty] & \text{if } m - \frac{d}{s} > 0, \\ [s, \infty) & \text{if } m - \frac{d}{s} = 0, \\ [s, -\frac{d}{m-(d/s)}] & \text{if } m - \frac{d}{s} < 0. \end{cases} \tag{2.8}$$

We also use the following Grönwall lemma: let $E(s) \in W^{1,1}(0, t)$ and $Q(s), P(s), R(s) \in L^1(0, t)$, where all functions are non-negative. Then,

$$\frac{dE}{ds} + P(s) \leqslant R(s)E(s) + Q(s) \quad \text{a.e. in } [0, t] \tag{2.9}$$

implies

$$E(t) + \int_0^t P(\tau)\,d\tau \leqslant e^{A(t)}E(0) + e^{A(t)}\int_0^t Q(\tau)\,d\tau, \tag{2.10}$$

where $A(t) := \int_0^t R(\tau)d\tau$.

For later use we recall the simple Young's inequality:

$$ab \leqslant \frac{\varepsilon}{2}a^2 + \frac{1}{2\varepsilon}b^2, \quad \forall a, b, \varepsilon > 0. \tag{2.11}$$

A more general Young's inequality is the following: for any $\varepsilon > 0$, $a, b \geqslant 0$, and $m, n > 1$

$$ab \leqslant \varepsilon^{m/n}\frac{a^m}{m} + \frac{1}{\varepsilon}\frac{b^n}{n}, \qquad \frac{1}{m} + \frac{1}{n} = 1. \tag{2.12}$$

Throughout we let C denote a finite, positive constant, independent of the mesh parameters, possibly depending on T, Ω, u_0 and v_0.

3 A semi-discrete approximation

Initially, we discuss results and assumptions associated with the finite element spaces.

3.1 Preliminaries

Consider the finite element approximation of (P_1) with the following mesh assumptions:

($\mathbf{A}^h$) Let $\Omega \subset \mathbb{R}^d$, $d \leqslant 3$, be a convex polygonal domain if $d = 2$ and a convex polyhedral domain if $d = 3$. Let $\mathscr{T}^h$ be a quasi-uniform partitioning [13, p.132] of Ω into disjoint open simplices $\{\tau\}$ with $h_\tau := \operatorname{diam}\tau$ and $h := \max_{\tau\in\mathscr{T}^h} h_\tau$, so that $\overline{\Omega} = \cup_{\tau\in\mathscr{T}^h}\overline{\tau}$. Additionally, we assume $\mathscr{T}^h$ is weakly acute (e.g. see Elliott [18] and Nochetto [33, p.49], that is in the case $d = 2$, for any pair of adjacent triangles the sum of the opposite angles relative to the common side does not exceed π, and in the case $d = 3$, the angle made by any two faces of the same tetrahedron does not exceed $\pi/2$.

Let $S^h \subset H^1(\Omega)$ be the standard finite element space of continuous functions on $\overline{\Omega}$ that are linear on each $\tau \in \mathscr{T}^h$. Let $\{\varphi_j\}_{j=0}^J$ be the canonical basis associated with S^h, satisfying $\varphi_j(x_i) = \delta_{ij}$, where $\{x_i\}_{i=0}^J$ is the set of nodes of $\mathscr{T}^h$. Let $\pi^h : C(\overline{\Omega}) \mapsto S^h$ be the Lagrange interpolation operator such that $\pi^h v(x_j) = v(x_j)$ for all $j = 0, \ldots J$. We define a discrete L^2 inner product on $C(\overline{\Omega})$ via

$$(u, v)^h := \int_\Omega \pi^h(u(x)v(x))\, dx \equiv \sum_{j=0}^{J} \widehat{M}_{jj} u(x_j) v(x_j), \tag{3.1}$$

[13, p.182], where $\widehat{M}_{jj} := (1, \varphi_j) \equiv (\varphi_j, \varphi_j)^h > 0$. It is easy to verify that $(\pi^h\eta, \chi)^h = (\eta, \chi)^h$, $\forall \eta, \chi \in C(\overline{\Omega})$. For future reference we also define

$$M_{ij} := (\varphi_i, \varphi_j), \quad K_{ij} := (\nabla\varphi_i, \nabla\varphi_j), \quad \widehat{M}_{ij} := (\varphi_i, \varphi_j)^h, \tag{3.2}$$

corresponding to the the mass matrix M, stiffness matrix K and lumped mass matrix $\widehat{M}$ respectively. From the above-mentioned references, as the partitioning $\mathscr{T}^h$ is weakly acute we have

$$\text{(i)} \sum_{j=0}^{J} K_{ij} \geqslant 0 \quad \forall i, \quad \text{(ii)}\, K_{ij} \leqslant 0 \quad (i \neq j). \tag{3.3}$$

In fact, it follows directly for our method that $\sum_{j=0}^{J} K_{ij} = 0$.

The following lemma will be important in deriving stability estimates and is a consequence of the weak acuteness property (3.3) (for a proof see Garvie [20, Lemma 4.2.1]).

Lemma 3.1 (Discrete Maximum Principle) *Assume the partitioning $\mathscr{T}^h$ is weakly acute and* $\mathbf{U}$ *is a monotone function on* $\mathbb{R}^n$*,* $n \in \mathbb{N}$*, then*

$$(\nabla \boldsymbol{\chi}^h, \nabla \pi^h \mathbf{U}(\boldsymbol{\chi}^h)) \geqslant 0, \qquad \forall \boldsymbol{\chi}^h \in \{S^h\}^n.$$

It is well-known that the discrete inner product (3.1) induces a norm on $S^h \subset C(\overline{\Omega})$ via $|\chi^h|_h := \sqrt{(\chi^h, \chi^h)^h}, \quad \forall \chi^h \in S^h$, and $\|\cdot\|_0$ and $|\cdot|_h$ are equivalent norms, i.e.

$$c\|\chi^h\|_0 \leqslant |\chi^h|_h \leqslant C\|\chi^h\|_0, \quad \forall \chi^h \in S^h,$$

[36, 35]), where c and C are independent of h. We shall make frequent use of this result without referring to it. We generalise the discrete norm above and introduce new discrete L^p spaces and associated results that allow us to smoothly carry over many continuous results to the discrete setting. For all $\chi^h \in S^h$ and $1 \leqslant p < \infty$ define:

$$|\chi^h|_{h,p} := \left(\int_\Omega \pi^h \{|\chi^h(x)|^p\}\, dx \right)^{1/p} \equiv \left(\sum_{j=0}^{J} \widehat{M}_{jj} |\chi^h(x_j)|^p \right)^{1/p}, \tag{3.4a}$$

$$\text{and} \qquad |\chi^h|_{h,\infty} := \max_{0 \leqslant j \leqslant J} |\chi^h(x_j)| \quad \text{if } p = \infty. \tag{3.4b}$$

Using the standard discrete Hölder and Minkowski inequalities [31, pp. 271–274], it is easy to prove the following discrete Minkowski and Hölder inequalities for all $u, v \in C(\overline{\Omega})$ (and hence also for elements in S^h):

$$|u + v|_{h,p} \leqslant |u|_{h,p} + |v|_{h,p}, \quad 1 \leqslant p \leqslant \infty, \tag{3.5}$$

$$|(u, v)^h| \leqslant |u|_{h,p} |v|_{h,q}, \quad \frac{1}{p} + \frac{1}{q} = 1, \quad 1 \leqslant p, q \leqslant \infty. \tag{3.6}$$

Using (3.5) it is easy to verify that (3.4a)–(3.4b) is a norm on S^h (*not* $C(\overline{\Omega})$), and we denote the Banach space $L^{h,p}(\Omega)$ to be the space S^h equipped with the norm $|\cdot|_{h,p}$ for $1 \leqslant p \leqslant \infty$. In addition to the discrete Hölder and Minkowski inequalities we have a simple injection result:

$$|\chi^h|_{h,q} \leqslant C|\chi^h|_{h,p}, \quad C = |\Omega|^{1/q - 1/p}, \quad 1 \leqslant q \leqslant p \leqslant \infty, \quad \forall \chi^h \in L^{h,p}(\Omega). \tag{3.7}$$

We extend these finite-dimensional spaces to time-dependent ones $L^{h,p}(\Omega_T)$, with norm

$$|\chi^h|_{h,p,\Omega_T} := \left(\int_0^T |\chi^h(\cdot,t)|^p_{h,p}\, dt \right)^{1/p}, \quad 1 \leqslant p \leqslant \infty, \quad \forall \chi^h \in S^h, \tag{3.8}$$

which is the discrete analogue of $L^p(\Omega_T) \equiv L^p(0,T;L^p(\Omega))$, satisfying $\forall \chi^h \in L^{h,p}(\Omega_T)$

$$|\chi^h|_{h,q,\Omega_T} \leqslant C|\chi^h|_{h,p,\Omega_T}, \quad C = (|\Omega|T)^{1/q-1/p}, \quad 1 \leqslant q \leqslant p \leqslant \infty. \tag{3.9}$$

We require the following well-known interpolation error estimates (see Ciarlet & Raviart [14, Theorem 5]):

$$\|(I-\pi^h)\chi\|_0 + h|(I-\pi^h)\chi|_1 \leqslant Ch^2|\chi|_2, \quad \forall \chi \in H^2(\Omega), \quad d \leqslant 3, \tag{3.10a}$$

$$\|(I-\pi^h)\chi\|_{0,1} \leqslant Ch^2|\chi|_{2,1}, \quad \forall \chi \in W^{2,1}(\Omega), \quad d \leqslant 3, \tag{3.10b}$$

the inverse estimates (see Ciarlet [13, Theorem 3.2.6.]) for all $\chi^h \in S^h$

$$|\chi^h|_1 \leqslant \frac{C}{h}|\chi^h|_h, \tag{3.11a}$$

$$\|\chi^h\|_{0,q} \leqslant Ch^{d(1/q-1/r)}\|\chi^h\|_{0,r}, \quad 1 \leqslant r \leqslant q \leqslant \infty, \tag{3.11b}$$

$$|\chi^h|_{1,q} \leqslant Ch^{d(1/q-1/r)}|\chi^h|_{1,r}, \quad 1 \leqslant r \leqslant q \leqslant \infty, \tag{3.11c}$$

expressions for the error due to numerical integration

$$|(\chi^h,\eta^h) - (\chi^h,\eta^h)^h| \leqslant Ch^2|\chi^h|_1|\eta^h|_1, \quad \forall \chi^h,\eta^h \in S^h, \tag{3.12a}$$

$$|(\chi^h,\eta^h) - (\chi^h,\eta^h)^h| \leqslant Ch\|\chi^h\|_0|\eta^h|_1, \quad \forall \chi^h,\eta^h \in S^h, \tag{3.12b}$$

(see Thomée [41, Lemma 15.1]), and a result for the L^2 projection operator $P^h : L^2(\Omega) \mapsto S^h$ satisfying $(P^h\eta,\chi^h) = (\eta,\chi^h)$, $\forall \chi^h \in S^h$ (e.g. see Barrett *et al.* [7, 8]), namely,

$$\|(I-P^h)\eta\|_0 + h|(I-P^h)\eta|_1 \leqslant Ch^m|\eta|_m, \quad m = 1,2 \quad \forall \eta \in H^m(\Omega). \tag{3.13}$$

We present several theorems that are the discrete analogues of continuous theorems.

Lemma 3.2 (Discrete Sobolev embedding) *Let $v \in S^h$, $r \in \mathbb{R}$, $h \leqslant 1$ and assume the triangulation $\mathcal{T}^h$ is quasi-uniform, then there exists a positive constant C such that*

$$|v|_{h,r} \leqslant C\|v\|_1 \quad \textit{holds for} \quad r \in \begin{cases} [2,\infty] & \textit{if } d = 1, \\ [2,\infty) & \textit{if } d = 2, \\ [2,6] & \textit{if } d = 3. \end{cases} \tag{3.14}$$

Proof Let τ be a fixed simplex, $v \in S^h$, and $r \geqslant 2$. As $C^{r-1,1}(\bar{\Omega}) \hookrightarrow W^{2,1}(\Omega)$ (see the comment after Theorem 5.1 in Rodrigues [38]) we take $\chi = |v|^r \in C^{r-1,1}(\bar{\Omega})$ in (3.10*b*), note that χ is differentiable r times a.e. on τ, yielding

$$\frac{\partial^2 |v|^r}{\partial x_i \partial x_j} = r(r-1)\frac{\partial v}{\partial x_i}\frac{\partial v}{\partial x_j}|v|^{r-2} \quad \text{a.e. on } \tau.$$

Thus with application of the Cauchy-Schwarz inequality we have

$$\int_\tau \left|(I-\pi^h)|v|^r\right| dx \leqslant Ch_\tau^2 \sum_{|\alpha|=2} \int_\tau |D^\alpha |v|^r|\, dx \leqslant Ch^2 \|v\|_{L^\infty(\tau)}^{r-2} |v|_{H^1(\tau)}^2.$$

Adding the contributions from all simplices leads to

$$\int_\Omega \left|(I-\pi^h)|v|^r\right| dx \leqslant Ch^2 \|v\|_{0,\infty}^{r-2} |v|_1^2. \tag{3.15}$$

Application of the standard Sobolev embedding theorem and the inverse inequality (3.11*b*) yields

$$\int_\Omega |(I-\pi^h)|v|^r|\, dx \leqslant \begin{cases} Ch^2 \|v\|_1^r \text{ if } d=1, \\ Ch^{2+\frac{2(2-r)}{p}} \|v\|_1^r \quad \forall p \in [2,\infty) \text{ if } d=2, \\ Ch^{3-\frac{r}{2}} \|v\|_1^r \text{ if } d=3. \end{cases} \tag{3.16}$$

Split $\quad |v|_{h,r}^r \leqslant \|(I-\pi^h)|v|^r\|_{0,1} + \|v\|_{0,r}^r$

$$\leqslant \begin{cases} C(h^2+1)\|v\|_1^r,\ r \in [2,\infty] \text{ if } d=1, \\ C\left(h^{2+\frac{2(2-r)}{p}}+1\right)\|v\|_1^r,\ r,p \in [2,\infty) \text{ if } d=2, \\ C\left(h^{3-\frac{r}{2}}+1\right)\|v\|_1^r,\ r \in [2,6] \text{ if } d=3, \end{cases}$$

where again, we used the Sobolev embedding theorem. To obtain constants independent of h note $h^\alpha < |\Omega|^\alpha$ if $\alpha \in \mathbb{R}^+$ and the restrictions on r. □

Lemma 3.3 (Discrete Gagliardo-Nirenberg) *Let $v \in S^h$, $r \in \mathbb{R}$, $h \leqslant 1$, $\mu := d\left(\frac{1}{2}-\frac{1}{r}\right)$ and assume the triangulation $\mathscr{T}^h$ is quasi-uniform, then*

$$|v|_{h,r} \leqslant \frac{C}{h} |v|_h^{1-\mu} \|v\|_1^\mu, \tag{3.17}$$

with the same restrictions on r as in (3.14).

The proof follows readily from Lemma 3.2, the inverse inequality (3.11*a*), $L^r \hookrightarrow L^2$ ($r \geqslant 2$), and the Gagliardo-Nirenberg inequality (2.8) with $m=1$.

Lemma 3.4 *Assume ρ and ε are non-negative real numbers, ρ satisfies assumption* (A1) *and $\eta, \psi \in S^h$, $h \leqslant 1$ and the triangulation $\mathscr{T}^h$ is quasi-uniform. Then there are constants $C_h(\varepsilon) := C(\varepsilon)h^{2/(\mu-1)} > 0$, $\mu := d(\frac{1}{2}-\frac{1}{\rho+2})$ and C such that*

$$C\left(|\eta|^\rho, |\psi|^2\right)^h \leqslant \left(\frac{\mu}{\varepsilon} + C_h(\varepsilon)|\eta|_{h,\rho+2}^{\frac{\rho}{1-\mu}}\right)\|\psi\|_0^2 + \frac{\mu}{\varepsilon}|\psi|_1^2, \quad \textit{where } 0<\mu<1. \tag{3.18}$$

The proof is the discrete analogue of the proof of Lemma 3.2 in [11] and relies on (3.6), (3.17) and (2.12).

We give two equivalent semi-discrete approximations of (P_1) and (P_2) respectively:

($\mathbf{P}_1^h$) Find $\mathbf{u}^h(\cdot,t) \in \{S^h\}^2$ such that $\mathbf{u}^h(\cdot,0) = P^h\mathbf{u}_0(\cdot)$ and for a.e. $t \in (0,T)$

$$(\mathbf{u}_t^h, \boldsymbol{\chi}^h)^h + (\nabla \mathbf{u}^h, \nabla \boldsymbol{\chi}^h) = (B\mathbf{u}^h, \boldsymbol{\chi}^h)^h + (|\mathbf{u}^h|^\rho A\mathbf{u}^h, \boldsymbol{\chi}^h)^h \quad \forall \boldsymbol{\chi}^h \in \{S^h\}^2, \tag{3.19}$$

where $\mathbf{u}^h := (u^h, v^h)^T$.

($\mathbf{P}_2^h$) Find $c^h(\cdot,t) \in \mathbb{S}^h$ such that $c^h(\cdot,0) = P^h c_0(\cdot)$ and for a.e. $t \in (0,T)$

$$(c_t^h, \chi^h)^h + (\nabla c^h, \nabla \chi^h) = (\lambda(r^h)c^h, \chi^h)^h + i(\omega(r^h)c^h, \chi^h)^h \quad \forall \chi^h \in \mathbb{S}^h,$$

where $c^h := u^h + iv^h$, $r^h \equiv |c^h|$ and $\mathbb{S}^h$ is the 'complexified' space of S^h, i.e. if $c = c_1 + i\,c_2 \in \mathbb{S}^h$ then $c_j \in S^h$, $j = 1,2$.

Lemma 3.5 *Let the assumptions* (A1) *and* (A^h) *hold,* $u_0, v_0 \in H^1(\Omega)$ *and* $h \leqslant 1$. *Then* (P_1^h) *possesses a unique solution* $\{u^h, v^h\}$ *such that the following stability bounds hold independent of* h*:*

$$u^h, v^h \in L^\infty(0,T; H^1(\Omega)) \cap L^{h,2\rho+2}(\Omega_T), \tag{3.20}$$

$$\frac{\partial u^h}{\partial t}, \frac{\partial v^h}{\partial t} \in L^2(\Omega_T). \tag{3.21}$$

Proof We prove separately: local existence of the approximations, global existence of the approximations, uniqueness, and an additional stability estimate.

Local existence of the semi-discrete approximations

In (P_2^h) let $c^h(\cdot,t) = \sum_{i=0}^J C_i(t)\varphi_i(\cdot)$ where $C_i(t) \approx c(x_i,t)$ and take $\chi^h = \varphi_j$, $j = 0,\dots,J$ yielding the following system of $(J+1)$ complex ordinary differential equations (ODEs):

$$\widehat{M}\frac{d\mathbf{C}}{dt} + K\mathbf{C} = \widehat{M}\mathbf{f}(\mathbf{C}), \quad \mathbf{c}^0 := M\mathbf{C}(0),$$

where $\mathbf{C} := (C_0,\dots,C_J)^T$, $\{\mathbf{c}^0\}_i := (c_0,\varphi_i)$, $\{\mathbf{f}(\mathbf{C})\}_i := f(C_i)$. We simplify this system by writing $f(C_i) = \widehat{f}(C_i)C_i$ where $\widehat{f}(C_i) := \lambda(R_i) + i\omega(R_i)$, $R_i \equiv |C_i|$, so that $\mathbf{f}(\mathbf{C}) = D\mathbf{C}$, $D := \mathrm{diag}\{\widehat{f}(C_0),\dots,\widehat{f}(C_J)\}$. $\widehat{M}$ is non-singular, so the above system becomes

$$\frac{d\mathbf{C}}{dt} = (D - \widehat{K})\mathbf{C}, \quad \mathbf{C}(0) = M^{-1}\mathbf{c}^0,$$

where $\widehat{K} := (\widehat{M})^{-1}K$. As f is a locally Lipschitz function (see (2.6)) from standard existence theory for systems of ODEs this system has a unique solution $\mathbf{C}$ (and hence (P_2^h) has a unique solution c^h) on some finite time interval $(0,t_h)$, $t_h > 0$.

3.2 Global existence of the semi-discrete approximations

To obtain global existence of the approximations we derive an *a priori* estimate bounding u^h, v^h independent of h, thus concluding $t_h = T$ (T independent of h).

Estimate I The estimate is a discrete analogue of (a generalised version) of Estimate I in Blowey & Garvie [11]. Choosing $\boldsymbol{\chi}^h = \pi^h\{|\mathbf{u}^h|^m\mathbf{u}^h\}$, $m \geqslant 0$, in (P_1^h) leads to

$$\frac{1}{(m+2)}\frac{d}{dt}|\mathbf{u}^h|_{h,m+2}^{m+2} + \lambda_1|\mathbf{u}^h|_{h,\rho+m+2}^{\rho+m+2} \leqslant \lambda_0|\mathbf{u}^h|_{h,m+2}^{m+2}, \tag{3.22}$$

after noting $|\mathbf{u}^h|^m\mathbf{u}^h\cdot\frac{\partial\mathbf{u}^h}{\partial t} = \frac{1}{(m+2)}\frac{\partial}{\partial t}|\mathbf{u}^h|^{m+2}$, Lemma 3.1 and (2.2*a*). Multiplying (3.22) through by $(m+2)$ and applying the Grönwall lemma yields for a.e. $t \in (0, T)$

$$|\mathbf{u}^h(t)|_{h,m+2}^{m+2} + \lambda_1(m+2)\int_0^t |\mathbf{u}^h(s)|_{h,\rho+m+2}^{\rho+m+2}\,ds \leqslant |\mathbf{u}^h(0)|_{h,m+2}^{m+2}\,e^{\lambda_0(m+2)t}. \tag{3.23}$$

We bound the right-hand side of (3.23) with $m = \rho$. Noting assumption (A1), Lemma 3.2, the projection property (3.13) and the fact that the initial data is in $H^1(\Omega)$ yields

$$|P^h\mathbf{u}_0|_{h,\rho+2}^{\rho+2} \leqslant C\|P^h\mathbf{u}_0\|_1^{\rho+2} \leqslant C\|\mathbf{u}_0\|_0^{\rho+2} + C|(I-P^h)\mathbf{u}_0|_1^{\rho+2} + C|\mathbf{u}_0|_1^{\rho+2} \leqslant C, \tag{3.24}$$

thus the following bounds hold independent of h:

$$u^h, v^h \in L^{h,2\rho+2}(\Omega_T) \cap L^\infty(0,T;L^{h,\rho+2}(\Omega)). \tag{3.25}$$

3.3 Uniqueness

The proof is a discrete analogue of the corresponding proof in Blowey & Garvie [11]. Assume there exist two semi-discrete solutions $\mathbf{u}^h, \mathbf{v}^h$ of (P_1^h). Setting $\boldsymbol{\chi}^h = \mathbf{w}^h := \mathbf{u}^h - \mathbf{v}^h$ and subtracting semi-discrete approximations yield

$$\frac{1}{2}\frac{d}{dt}|\mathbf{w}^h|_h^2 + |\mathbf{w}^h|_1^2 = \lambda_0|\mathbf{w}^h|_h^2 + \left(|\mathbf{u}^h|^\rho A\mathbf{u}^h - |\mathbf{v}^h|^\rho A\mathbf{v}^h, \mathbf{w}^h\right)^h, \tag{3.26}$$

after noting (2.2*a*). We bound the last term in this equation using (2.6), Lemma 3.4 with $\eta \in \{\mathbf{u}^h, \mathbf{v}^h\}$ and $\varepsilon = 2$, (2.2*a*), and a uniform bound in (3.25) to give

$$\left(|\mathbf{u}^h|^\rho A\mathbf{u}^h - |\mathbf{v}^h|^\rho A\mathbf{v}^h, \mathbf{w}^h\right)^h \leqslant \widehat{C}_h\|\mathbf{w}^h\|_0^2 + \mu|\mathbf{w}^h|_1^2, \tag{3.27}$$

where $\widehat{C}_h > 0$ is a constant depending on h. As $\mu < 1$ and $k := \rho/(1-\mu)$, after kickback of $\mu|\mathbf{w}^h|_1^2$ with (3.26), (3.27), and application of the Grönwall lemma, we have $|\mathbf{w}(t)|_h^2 \leqslant |\mathbf{w}(0)|_h^2\exp(\widehat{C}_h t)$, for a.e. $t \in (0, T)$, leading to $\mathbf{u}^h \equiv \mathbf{v}^h$, as required.

3.4 An additional stability estimate

Estimate II This estimate is a discrete analogue of Estimate III in Blowey & Garvie [11]. Choosing $\boldsymbol{\chi}^h = \mathbf{u}_t^h$ in (P_1^h), noting $|\mathbf{u}^h|^\rho\frac{\partial}{\partial t}|\mathbf{u}^h|^2 = \frac{2}{(\rho+2)}\frac{\partial}{\partial t}|\mathbf{u}^h|^{\rho+2}$, (2.2*b*), a simple Young's inequality, rearranging and integrating over $(0,t)$ yields for a.e. $t \in (0,T)$

$$\int_0^t \left|\frac{\partial \mathbf{u}^h(s)}{\partial t}\right|_h^2 ds + |\mathbf{u}^h(t)|_1^2 + \frac{2\lambda_1}{(\rho+2)}|\mathbf{u}^h(t)|_{h,\rho+2}^{\rho+2} + \lambda_0|\mathbf{u}^h(0)|_h^2 \leqslant \lambda_0|\mathbf{u}^h(t)|_h^2 +$$
$$2\omega_0^2\int_0^t |\mathbf{u}^h(s)|_h^2\,ds + 2\omega_1^2\int_0^t |\mathbf{u}^h(s)|_{h,2\rho+2}^{2\rho+2}\,ds + |\mathbf{u}^h(0)|_1^2 + \frac{2\lambda_1}{(\rho+2)}|\mathbf{u}^h(0)|_{h,\rho+2}^{\rho+2}. \tag{3.28}$$

Applying the discrete injection results (3.7) and (3.9), and noting (3.24) and (3.25), we conclude that the right hand side of (3.28) is bounded uniformly. Thus from the injection $L^{h,\rho+2}(\Omega) \hookrightarrow L^{h,2}(\Omega)$, the H^1 semi-norm bound, and (3.25), we deduce that the bounds $u^h, v^h \in L^\infty(0,T;H^1(\Omega))$, $\frac{\partial u^h}{\partial t}, \frac{\partial v^h}{\partial t} \in L^2(\Omega_T)$ hold independent of h. □

Remark: The approach in Estimate I of taking the test function equal to the interpolant of a monotonic nonlinear function is non-standard, although it has been used previously in the numerical analysis of the Cahn–Hilliard equation [2, 5]. The benefit is increased 'regularity' of the semi-discrete approximations, allowing us to dispense with a discrete analogue of Estimate II in Blowey & Garvie [11].

3.5 A semi-discrete error estimate

We prove an error estimate between the solutions of problems (P_1) and (P_1^h), which is optimal in H^1, but sub-optimal in L^2. The classical approach for deriving a semi-discrete error bound is via an elliptic ('Ritz') projection, which can be traced back to Wheeler [42] (see also Thomée [41]). The elliptic Ritz projection method and duality techniques are mostly for linear problems where the source term f is smooth, and thus there is no advantage in using this theoretical set-up here. The technical difficulties in the error estimates for our problem are entirely due to the nonlinear terms. For these reasons instead of the elliptic Ritz projection we use the interpolant $\pi^h\mathbf{u}$, which facilitates handling of the nonlinearity [2, 3, 24].

Lemma 3.6 *Let the assumptions of Theorem 1.1, Lemma 3.5, and* (A3) *hold. Then the solution* $\{u^h, v^h\}$ *of* (P_1^h) *satisfies the following semi-discrete error bound:*

$$\|\mathbf{u}-\mathbf{u}^h\|_{L^\infty(0,T;L^2(\Omega))} + \|\mathbf{u}-\mathbf{u}^h\|_{L^2(0,T;H^1(\Omega))} \leqslant Ch. \tag{3.29}$$

Proof Define

$$\left.\begin{aligned} \mathbf{e} &:= \mathbf{u}-\mathbf{u}^h \\ \mathbf{e}^A &:= \mathbf{u}-\pi^h\mathbf{u} \\ \mathbf{e}^h &:= \pi^h\mathbf{u}-\mathbf{u}^h \end{aligned}\right\} \quad \text{so} \quad \mathbf{e} := \mathbf{e}^A + \mathbf{e}^h.$$

Note that $\pi^h\mathbf{u}$ is well-defined as from the Sobolev embedding theorem $H^2(\Omega) \hookrightarrow C(\overline{\Omega})$, $d \leqslant 3$ and $u(\cdot,t), v(\cdot,t) \in H^2(\Omega)$ for a.e. $t \in (0,T)$ (see Theorem 1.1). We choose $\boldsymbol{\eta} = \mathbf{e}^h$ in

(P_1), $\boldsymbol{\chi}^h = \mathbf{e}^h$ in (P_1^h) and subtract, yielding

$$(\mathbf{u}_t, \mathbf{e}^h) - (\mathbf{u}_t^h, \mathbf{e}^h)^h + (\nabla \mathbf{e}, \nabla \mathbf{e}^h) = (B\mathbf{u}, \mathbf{e}^h) - (B\mathbf{u}^h, \mathbf{e}^h)^h + (|\mathbf{u}|^\rho A\mathbf{u}, \mathbf{e}^h) - (|\mathbf{u}^h|^\rho A\mathbf{u}^h, \mathbf{e}^h)^h. \quad (3.30)$$

Adding and subtracting each of the terms $(B\mathbf{u}^h, \mathbf{e}^h)$, $(|\mathbf{u}^h|^\rho A\mathbf{u}^h, \mathbf{e}^h)$ and $(\mathbf{u}_t^h, \mathbf{e}^h)$ to (3.30) and rearranging leads to

$$\begin{aligned} \frac{1}{2}\frac{d}{dt}\|\mathbf{e}\|_0^2 + |\mathbf{e}|_1^2 &= \left\{(\mathbf{u}_t^h, \mathbf{e}^h)^h - (\mathbf{u}_t^h, \mathbf{e}^h)\right\} + \left(\frac{\partial \mathbf{e}}{\partial t}, \mathbf{e}^A\right) + (\nabla \mathbf{e}, \nabla \mathbf{e}^A) + (B\mathbf{e}, \mathbf{e}^h) \\ &+ \left\{(B\mathbf{u}^h, \mathbf{e}^h) - (B\mathbf{u}^h, \mathbf{e}^h)^h\right\} + (|\mathbf{u}|^\rho A\mathbf{u} - |\mathbf{u}^h|^\rho A\mathbf{u}^h, \mathbf{e}^h) \\ &+ \left\{(|\mathbf{u}^h|^\rho A\mathbf{u}^h, \mathbf{e}^h) - (|\mathbf{u}^h|^\rho A\mathbf{u}^h, \mathbf{e}^h)^h\right\} =: \sum_{i=1}^{7} T_i. \end{aligned} \quad (3.31)$$

We bound each term on the right-hand side of (3.31) separately. Using (3.12*b*), (3.10*a*) and the Young's inequality (2.11) with $\varepsilon = 8$ yields

$$T_1 = (\mathbf{u}_t^h, \mathbf{e}^h)^h - (\mathbf{u}_t^h, \mathbf{e}^h) \leqslant Ch^2\|\mathbf{u}_t^h\|_0^2 + \frac{1}{8}|\mathbf{e}|_1^2 + Ch^2\|\mathbf{u}\|_2^2. \quad (3.32)$$

With the aid of the Cauchy–Schwarz inequality and (3.10*a*) we have

$$T_2 \leqslant \left\|\frac{\partial \mathbf{e}}{\partial t}\right\|_0 \|\mathbf{e}^A\|_0 \leqslant Ch^2\|\mathbf{u}\|_2 \left\|\frac{\partial \mathbf{e}}{\partial t}\right\|_0, \quad (3.33)$$

and also noting the Young's inequality (2.11) with $\varepsilon = 8$, (3.10*a*), and the Cauchy–Schwarz inequality we have

$$T_3 \leqslant |\mathbf{e}|_1|\mathbf{e}^A|_1 \leqslant Ch\|\mathbf{u}\|_2|\mathbf{e}|_1 \leqslant Ch^2\|\mathbf{u}\|_2^2 + \frac{1}{16}|\mathbf{e}|_1^2. \quad (3.34)$$

From the Cauchy–Schwarz inequality, (2.2*b*), a Young's inequality, and (3.10*a*) we have

$$T_4 \leqslant C\|\mathbf{e}\|_0\|\mathbf{e}^h\|_0 \leqslant C\|\mathbf{e}\|_0^2 + Ch^4\|\mathbf{u}\|_2^2. \quad (3.35)$$

To bound the fifth term we use (3.12*b*), (2.2*b*), bound (3.20), the Young's inequality (2.11) with $\varepsilon = 8$ and (3.10*a*) to give

$$T_5 \leqslant |(B\mathbf{u}^h, \mathbf{e}^h) - (B\mathbf{u}^h, \mathbf{e}^h)^h| \leqslant Ch^2 + \frac{1}{8}|\mathbf{e}|_1^2 + Ch^2\|\mathbf{u}\|_2^2. \quad (3.36)$$

Using (2.6), a generalised Hölder inequality, the continuous injections $H^1 \hookrightarrow L^{3\rho}$, $H^1 \hookrightarrow L^6$, assumption (A3), Theorem 1.1, bound (3.20), the Young's inequality (2.11) with $\varepsilon = 8$, and (3.10*a*) leads to

$$T_6 \leqslant \int_\Omega \left||\mathbf{u}|^\rho A\mathbf{u} - |\mathbf{u}^h|^\rho A\mathbf{u}^h\right| |\mathbf{e}^h|\, dx \leqslant C\|\mathbf{e}\|_0^2 + \frac{1}{8}|\mathbf{e}|_1^2 + Ch^2\|\mathbf{u}\|_2^2. \quad (3.37)$$

Bounding the final term is more technical than the calculations for the previous terms.

First noting (3.10*b*) we have

$$T_7 \leqslant \int_\Omega \left|(I-\pi^h)|\mathbf{u}^h|^\rho A\mathbf{u}^h\cdot\mathbf{e}^h\right|\,dx \leqslant Ch^2\sum_{i,j=1}^d\int_\Omega\left|\frac{\partial^2(|\mathbf{u}^h|^\rho A\mathbf{u}^h\cdot\mathbf{e}^h)}{\partial x_i\partial x_j}\right|\,dx =: T_{7,1}. \tag{3.38}$$

To expand the right-hand side of (3.38) we need the following identities, which are easily verified for arbitrary differentiable vector valued functions $\boldsymbol{\psi}$, $\boldsymbol{\phi}$, $\boldsymbol{\eta}\in\mathbb{R}^2$ and all $p\in\mathbb{R}$:

$$\frac{\partial}{\partial x_k}|\boldsymbol{\psi}|^p = p|\boldsymbol{\psi}|^{p-2}\left(\boldsymbol{\psi}\cdot\frac{\partial\boldsymbol{\psi}}{\partial x_k}\right), \tag{3.39}$$

$$\frac{\partial}{\partial x_k}\left(|\boldsymbol{\psi}|^pA\boldsymbol{\phi}\cdot\boldsymbol{\eta}\right) = |\boldsymbol{\psi}|^p\left(A\boldsymbol{\phi}\cdot\frac{\partial\boldsymbol{\eta}}{\partial x_k}\right)+|\boldsymbol{\psi}|^p\left(\boldsymbol{\eta}\cdot A\frac{\partial\boldsymbol{\phi}}{\partial x_k}\right)+p|\boldsymbol{\psi}|^{p-2}\left(\boldsymbol{\psi}\cdot\frac{\partial\boldsymbol{\psi}}{\partial x_k}\right)(A\boldsymbol{\phi}\cdot\boldsymbol{\eta}). \tag{3.40}$$

We first evaluate $T_{7,1}$ over a fixed reference simplex τ. With the aid of (3.39), (3.40), (2.2*b*), and some lengthy, but elementary calculations we obtain

$$T_{7,1}^\tau := Ch_\tau^2\sum_{i,j=1}^d\int_\tau\left|\frac{\partial^2(|\mathbf{u}^h|^\rho A\mathbf{u}^h\cdot\mathbf{e}^h)}{\partial x_i\partial x_j}\right|\,dx$$

$$\leqslant Ch_\tau^2\sum_{i,j=1}^d\int_\tau\left\{|\mathbf{u}^h|^\rho\left|\frac{\partial\mathbf{e}^h}{\partial x_i}\right|\left|\frac{\partial\mathbf{u}^h}{\partial x_j}\right|+|\mathbf{u}^h|^\rho\left|\frac{\partial\mathbf{e}^h}{\partial x_j}\right|\left|\frac{\partial\mathbf{u}^h}{\partial x_i}\right|+|\mathbf{u}^h|^{\rho-1}\left|\frac{\partial\mathbf{u}^h}{\partial x_j}\right|\left|\frac{\partial\mathbf{u}^h}{\partial x_i}\right||\mathbf{e}^h|\right\}\,dx,$$

and
$$T_{7,1}\leqslant\sum_\tau T_{7,1}^\tau\leqslant Ch^2\sum_{i,j=1}^d\int_\Omega\left\{|\mathbf{u}^h|^\rho\left|\frac{\partial\mathbf{e}^h}{\partial x_i}\right|\left|\frac{\partial\mathbf{u}^h}{\partial x_j}\right|+|\mathbf{u}^h|^\rho\left|\frac{\partial\mathbf{e}^h}{\partial x_j}\right|\left|\frac{\partial\mathbf{u}^h}{\partial x_i}\right|\right.$$
$$\left.+\,|\mathbf{u}^h|^{\rho-1}\left|\frac{\partial\mathbf{u}^h}{\partial x_j}\right|\left|\frac{\partial\mathbf{u}^h}{\partial x_i}\right||\mathbf{e}^h|\right\}\,dx =: T_{7,2}. \tag{3.41}$$

To bound the right-hand side of (3.41) we use a generalised Hölder inequality, $\|\partial\zeta/\partial x_k\|_{0,3}\leqslant|\zeta|_{1,3}$ for all ζ in $W^{1,3}$, assumption (A3), the injections $H^1\hookrightarrow L^{3\rho}$, $H^1\hookrightarrow L^{6\rho-6}$, the inverse inequality (3.11*c*) in the form $|\chi^h|_{1,3}\leqslant Ch^{-d/6}|\chi^h|_{1,2}$, bound (3.20), (3.10*a*), and the simple Young's inequality (2.11) with $\varepsilon=8$ to obtain

$$T_{7,2}\leqslant Ch^2\sum_{i,j=1}^d\left\{\|\mathbf{u}^h\|_{0,3\rho}^\rho\left\|\frac{\partial\mathbf{u}^h}{\partial x_j}\right\|_{0,3}\left\|\frac{\partial\mathbf{e}^h}{\partial x_i}\right\|_{0,3}+\|\mathbf{u}^h\|_{0,3\rho}^\rho\left\|\frac{\partial\mathbf{u}^h}{\partial x_i}\right\|_{0,3}\left\|\frac{\partial\mathbf{e}^h}{\partial x_j}\right\|_{0,3}\right.$$
$$\left.+\;\|\mathbf{u}^h\|_{0,6\rho-6}^{\rho-1}\|\mathbf{e}^h\|_{0,6}\left\|\frac{\partial\mathbf{u}^h}{\partial x_i}\right\|_{0,3}\left\|\frac{\partial\mathbf{u}^h}{\partial x_j}\right\|_{0,3}\right\}$$
$$\leqslant Ch^{2-\frac{d}{3}}(\|\mathbf{e}\|_0+Ch\|\mathbf{u}\|_2)+Ch^{2-\frac{d}{3}}|\mathbf{e}|_1 =: T_{7,3}. \tag{3.42}$$

Thus from (3.31)–(3.38), (3.41), (3.42), a kickback of $\frac{1}{2}|\mathbf{e}|_1^2$, and noting that $h^{4-\frac{2d}{3}}\leqslant h^2$ as $h\leqslant 1$, $d\leqslant 3$, we have

$$\frac{d}{dt}\|\mathbf{e}\|_0^2+|\mathbf{e}|_1^2\leqslant C\left(\|\mathbf{e}\|_0^2+h^2\|\mathbf{u}_t^h\|_0^2+h^2\|\mathbf{u}\|_2^2+h^2\|\mathbf{u}\|_2\left\|\frac{\partial\mathbf{e}}{\partial t}\right\|_0+h^2\right). \tag{3.43}$$

From the Grönwall lemma, the Cauchy–Schwarz inequality, Theorem 1.1, bound (3.21), (3.13), and recalling that $u_0, v_0 \in H^1(\Omega)$ it follows that for a.e. $t \in (0, T)$

$$\|\mathbf{e}(t)\|_0^2 + \int_0^t |\mathbf{e}(s)|_1^2\, ds \leqslant Ch^2$$

and the result follows. □

4 A fully discrete approximation

4.1 Preliminaries

Lemma 4.1 (Discrete Grönwall lemma) *Assume* $w_n, \alpha_n, p_n \geqslant 0,\ 0 \leqslant \beta < 1$, *satisfy*

$$w_n + p_n \leqslant \alpha_n + \beta \sum_{k=0}^{n-1} w_{k+1}, \quad \forall n \geqslant 1, \tag{4.1a}$$

$$w_0 + p_0 \leqslant \alpha_0, \tag{4.1b}$$

where $\{\alpha_n\}$ *is non-decreasing. Then*

$$w_n + \frac{p_n}{1-\beta} \leqslant \left(\frac{\alpha_n - \beta w_0}{1-\beta}\right) \exp\left(\frac{n\beta}{1-\beta}\right). \tag{4.2}$$

This is a straightforward adaptation of Lemma 10.5 in Thomée [41] (see Garvie [20, Lemma 5.1.1]).

Let N be a positive integer and $\Delta t := T/N$ be the time step. We consider the following fully discrete, semi-implicit in time, finite element approximation of (P_1):

$(\mathbf{P}_1^{h,\Delta t})$ For $n = 1, \ldots, N$ find $\mathbf{U}^n \in \{S^h\}^2$ such that $\mathbf{U}^0 := P^h\mathbf{u}_0$ and $\forall \boldsymbol{\chi}^h \in \{S^h\}^2$

$$\left(\frac{\mathbf{U}^n - \mathbf{U}^{n-1}}{\Delta t}, \boldsymbol{\chi}^h\right)^h + (\nabla \mathbf{U}^n, \nabla \boldsymbol{\chi}^h) = (B\mathbf{U}^n, \boldsymbol{\chi}^h)^h + (|\mathbf{U}^{n-1}|^\rho A\mathbf{U}^n, \boldsymbol{\chi}^h)^h, \tag{4.3}$$

where $\mathbf{U}^n := (U^n, V^n)^T$.

Lemma 4.2 *Let the assumptions of Lemma 3.6 hold and* $\Delta t < \min\{1, \frac{1}{\lambda_0(2\rho+2)}\}$. *Then there exists a unique solution to* $(\mathrm{P}_1^{h,\Delta t})$ *such that*

$$\max_{1 \leqslant n \leqslant N} \|\mathbf{U}^n\|_1 \leqslant C, \tag{4.4}$$

$$\sum_{n=1}^N |\mathbf{U}^n - \mathbf{U}^{n-1}|_h^2 \leqslant C\Delta t, \tag{4.5}$$

$$\sum_{n=1}^N |\mathbf{U}^n - \mathbf{U}^{n-1}|_1^2 \leqslant C. \tag{4.6}$$

Proof We show initially existence and uniqueness, followed by two stability estimates.

4.2 Existence and uniqueness

The linear system ($\mathrm{P}_1^{h,\Delta t}$) can be written as a square matrix system and so existence of the fully discrete approximation follows from the well-known fact that for a square linear system existence is equivalent to uniqueness. To prove uniqueness assume there are two fully discrete solutions $\mathbf{U}^n, \mathbf{V}^n$ ($n \geqslant 1$), of ($\mathrm{P}_1^{h,\Delta t}$). We use proof by induction. Assume uniqueness of the approximation at time $t_{n-1} := (n-1)\Delta t$ and note that we have uniqueness at time t_0. Now setting $\chi^h = \mathbf{W}^n := \mathbf{U}^n - \mathbf{V}^n$, subtracting the fully discrete approximations and noting (2.2a), yields

$$\frac{1}{\Delta t}|\mathbf{W}^n|_h^2 + |\mathbf{W}^n|_1^2 + \lambda_1 \left(|\mathbf{U}^{n-1}|^\rho, |\mathbf{W}^n|^2\right)^h = \lambda_0 |\mathbf{W}^n|_h^2. \tag{4.7}$$

By assumption $\lambda_0 < 1/\Delta t$ so $C(\Delta t)|\mathbf{W}^n|_h^2 + |\mathbf{W}^n|_1^2 \leqslant 0$, where $C(\Delta t)$ is a positive constant depending on Δt. We thus conclude $\mathbf{U}^n \equiv \mathbf{V}^n$ for all $n \geqslant 1$ as required.

4.3 Stability estimates

Estimate III The estimate is a fully discrete analogue of Estimate I. Choosing $\chi^h = \pi^h\{|\mathbf{U}^n|^m \mathbf{U}^n\}$, $m \geqslant 0$, in ($\mathrm{P}_1^{h,\Delta t}$) and noting Lemma 3.1, and (2.2a) lead to

$$\frac{1}{\Delta t}(|\mathbf{U}^n|^m, \mathbf{U}^n \cdot (\mathbf{U}^n - \mathbf{U}^{n-1}))^h + \lambda_1(|\mathbf{U}^{n-1}|^\rho, |\mathbf{U}^n|^{m+2})^h \leqslant \lambda_0 |\mathbf{U}^n|_{h,m+2}^{m+2}. \tag{4.8}$$

Applying the monotonicity property (2.7) to the first term in (4.8) and multiplying through by $\Delta t(m+2)$ lead to

$$|\mathbf{U}^n|_{h,m+2}^{m+2} - |\mathbf{U}^{n-1}|_{h,m+2}^{m+2} + \lambda_1 \Delta t(m+2)(|\mathbf{U}^{n-1}|^\rho, |\mathbf{U}^n|^{m+2})^h \leqslant \lambda_0 \Delta t(m+2)|\mathbf{U}^n|_{h,m+2}^{m+2}. \tag{4.9}$$

Summing both sides of (4.9) from $n = 1, \ldots, N$ yields

$$\begin{aligned} &|\mathbf{U}^N|_{h,m+2}^{m+2} + \lambda_1 \Delta t(m+2) \sum_{n=1}^{N} (|\mathbf{U}^{n-1}|^\rho, |\mathbf{U}^n|^{m+2})^h \\ &\quad \leqslant |\mathbf{U}^0|_{h,m+2}^{m+2} + \lambda_0 \Delta t(m+2) \sum_{n=0}^{N-1} |\mathbf{U}^{n+1}|_{h,m+2}^{m+2}. \end{aligned} \tag{4.10}$$

Applying the discrete Grönwall lemma to (4.10) for $\Delta t < \frac{1}{\lambda_0(m+2)}$ gives

$$\begin{aligned} &|\mathbf{U}^N|_{h,m+2}^{m+2} + \left(\frac{\lambda_1 \Delta t(m+2)}{1 - \lambda_0 \Delta t(m+2)}\right) \sum_{n=1}^{N} (|\mathbf{U}^{n-1}|^\rho, |\mathbf{U}^n|^{m+2})^h \\ &\quad \leqslant |\mathbf{U}^0|_{h,m+2}^{m+2} \exp\left(\frac{\lambda_0(m+2)T}{1 - \lambda_0 \Delta t(m+2)}\right), \quad (T \equiv N\Delta t). \end{aligned} \tag{4.11}$$

We choose $m = 2\rho$ in (4.11). With assumption (A2), Lemma 3.2 and (3.13) we have $|\mathbf{U}^0|_{h,2\rho+2}^{2\rho+2} \leqslant C$ (cf. (3.24)), leading to the following stability bound:

$$\max_{1 \leqslant n \leqslant N} |\mathbf{U}^n|_{h,2\rho+2} \leqslant C. \tag{4.12}$$

From (3.7) it follows that $|\mathbf{U}^N|_h \leqslant C|\mathbf{U}^N|_{h,2\rho+2}$ and hence we also have

$$\max_{1\leqslant n\leqslant N} |\mathbf{U}^n|_h \leqslant C. \tag{4.13}$$

Estimate IV The estimate is a fully discrete analogue of Estimate II. Choosing $\boldsymbol{\chi}^h = (\mathbf{U}^n - \mathbf{U}^{n-1})/\Delta t$ in $(\mathrm{P}_1^{h,\Delta t})$ leads to

$$\begin{aligned}\left|\frac{\mathbf{U}^n - \mathbf{U}^{n-1}}{\Delta t}\right|_h^2 &+ \frac{1}{2\Delta t}\left(|\mathbf{U}^n - \mathbf{U}^{n-1}|_1^2 + |\mathbf{U}^n|_1^2 - |\mathbf{U}^{n-1}|_1^2\right)\\ &= \left(B\mathbf{U}^n + |\mathbf{U}^{n-1}|^\rho A\mathbf{U}^n, \frac{\mathbf{U}^n - \mathbf{U}^{n-1}}{\Delta t}\right)^h,\end{aligned} \tag{4.14}$$

where we have used the elementary identity $2b(b-a) \equiv |b-a|^2 + b^2 - a^2$, $\forall a, b \in \mathbb{R}$. We apply a simple Young's inequality to the last term in (4.14) after noting (2.2*b*) to give

$$\begin{aligned}\left(B\mathbf{U}^n + |\mathbf{U}^{n-1}|^\rho A\mathbf{U}^n, \frac{\mathbf{U}^n - \mathbf{U}^{n-1}}{\Delta t}\right)^h &\leqslant \left(|B\mathbf{U}^n + |\mathbf{U}^{n-1}|^\rho A\mathbf{U}^n|, \left|\frac{\mathbf{U}^n - \mathbf{U}^{n-1}}{\Delta t}\right|\right)^h\\ &\leqslant C|\mathbf{U}^n|_h^2 + C(|\mathbf{U}^{n-1}|^{2\rho}, |\mathbf{U}^n|^2)^h + \frac{1}{2}\left|\frac{\mathbf{U}^n - \mathbf{U}^{n-1}}{\Delta t}\right|_h^2.\end{aligned} \tag{4.15}$$

Thus from (4.14), (4.15) and a kickback of $\frac{1}{2}|(\mathbf{U}^n - \mathbf{U}^{n-1})/\Delta t|_h^2$ we have

$$\begin{aligned}\left|\frac{\mathbf{U}^n - \mathbf{U}^{n-1}}{\Delta t}\right|_h^2 &+ \frac{1}{\Delta t}\left(|\mathbf{U}^n - \mathbf{U}^{n-1}|_1^2 + |\mathbf{U}^n|_1^2 - |\mathbf{U}^{n-1}|_1^2\right)\\ &\leqslant C|\mathbf{U}^n|_h^2 + C|\mathbf{U}^{n-1}|_{h,2\rho+2}^{2\rho}|\mathbf{U}^n|_{h,2\rho+2}^2 \leqslant C,\end{aligned} \tag{4.16}$$

where we used (3.6), and the stability bounds (4.12) and (4.13). Multiplying (4.16) through by Δt, summing from $n = 1, \ldots, N$, rearranging, and noting (3.13) lead to

$$\Delta t \sum_{n=1}^N \left|\frac{\mathbf{U}^n - \mathbf{U}^{n-1}}{\Delta t}\right|_h^2 + \sum_{n=1}^N |\mathbf{U}^n - \mathbf{U}^{n-1}|_1^2 + |\mathbf{U}^N|_1^2 \leqslant C.$$

Lemma 4.2 follows easily on noting (4.13). □

4.4 A fully discrete error bound

We prove an error estimate between the solutions of (P_1) and $(\mathrm{P}_1^{h,\Delta t})$ with no additional assumptions. For notational convenience we extend the fully discrete solutions via the piecewise-linear interpolant, or the piecewise-constant interpolant in time.

Theorem 4.1 *Let the assumptions of Lemma 4.2 hold. Then we have*

$$\|\mathbf{u}-\mathbf{U}^{+}\|_{L^{\infty}(0,T;L^{2}(\Omega))}+\|\mathbf{u}-\mathbf{U}^{+}\|_{L^{2}(0,T;H^{1}(\Omega))}\leqslant C(\Delta t^{1/2}+h), \tag{4.17}$$

$$\textit{where}\quad \mathbf{U}(t):=\left(\frac{t-t_{n-1}}{\Delta t}\right)\mathbf{U}^{n}+\left(\frac{t_{n}-t}{\Delta t}\right)\mathbf{U}^{n-1},\quad t\in[t_{n-1},t_{n}],\ n\geqslant 1,$$

$$\textit{and}\quad \mathbf{U}^{+}(t):=\mathbf{U}^{n},\quad \mathbf{U}^{-}(t):=\mathbf{U}^{n-1},\quad t\in(t_{n-1},t_{n}],\ n\geqslant 1. \tag{4.18}$$

Proof We note for future reference that

$$\frac{\partial\mathbf{U}}{\partial t}=\frac{\mathbf{U}^{+}-\mathbf{U}^{-}}{\Delta t}=\frac{\mathbf{U}-\mathbf{U}^{-}}{t-t_{n-1}}=\frac{\mathbf{U}^{+}-\mathbf{U}}{t_{n}-t},\quad t\in(t_{n-1},t_{n}],\ n\geqslant 1. \tag{4.19}$$

We restate $(\mathrm{P}_{1}^{h,\Delta t})$ as follows:

Find $\mathbf{U}\in\{H^{1}(0,T;S^{h})\}^{2}$ such that $\mathbf{U}(\cdot,0):=P^{h}\mathbf{u}_{0}(\cdot)$ and for a.e. $t\in(0,T)$

$$\left(\frac{\partial\mathbf{U}}{\partial t},\boldsymbol{\chi}^{h}\right)^{h}+(\nabla\mathbf{U}^{+},\nabla\boldsymbol{\chi}^{h})=(B\mathbf{U}^{+},\boldsymbol{\chi}^{h})^{h}+(|\mathbf{U}^{-}|^{\rho}A\mathbf{U}^{+},\boldsymbol{\chi}^{h})^{h}\quad\forall\boldsymbol{\chi}^{h}\in\{S^{h}\}^{2}. \tag{4.20}$$

Define $\mathbf{E}^{+}:=\mathbf{u}^{h}-\mathbf{U}^{+}\in\{S^{h}\}^{2}$, $\mathbf{E}:=\mathbf{u}^{h}-\mathbf{U}\in\{S^{h}\}^{2}$ and $\mathbf{E}^{-}:=\mathbf{u}^{h}-\mathbf{U}^{-}\in\{S^{h}\}^{2}$, so that $\mathbf{E}^{+}-\mathbf{E}\equiv\mathbf{U}-\mathbf{U}^{+}\equiv(t-t_{n})\frac{\partial\mathbf{U}}{\partial t}$ and $\mathbf{E}^{-}-\mathbf{E}\equiv\mathbf{U}-\mathbf{U}^{-}\equiv\Delta t\frac{\partial\mathbf{U}}{\partial t}$. Choose $\boldsymbol{\chi}^{h}=\mathbf{E}^{+}$ in (4.20) and (3.19), and subtract, which after noting (2.2*a*) lead to

$$\left(\frac{\partial\mathbf{E}}{\partial t},\mathbf{E}^{+}\right)^{h}+|\mathbf{E}^{+}|_{1}^{2}=\lambda_{0}|\mathbf{E}^{+}|_{h}^{2}+(|\mathbf{u}^{h}|^{\rho}A\mathbf{u}^{h}-|\mathbf{U}^{-}|^{\rho}A\mathbf{U}^{+},\mathbf{E}^{+})^{h},\quad\text{where }\mathbf{E}(0)=0.$$

We rewrite this as

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}|\mathbf{E}|_{h}^{2}+|\mathbf{E}^{+}|_{1}^{2}&=\left(\frac{\partial\mathbf{E}}{\partial t},\mathbf{U}^{+}-\mathbf{U}\right)^{h}+\lambda_{0}|\mathbf{E}^{+}|_{h}^{2}+(|\mathbf{u}^{h}|^{\rho}A\mathbf{u}^{h}-|\mathbf{U}^{-}|^{\rho}A\mathbf{U}^{+},\mathbf{E}^{+})^{h}\\&\equiv I_{1}+I_{2}+I_{3}.\end{aligned} \tag{4.21}$$

Noting (3.6) and (4.19) we have after simplification

$$I_{1}\leqslant\left|\frac{\partial\mathbf{E}}{\partial t}\right|_{h}|\mathbf{U}^{+}-\mathbf{U}|_{h}\leqslant\left|\frac{\partial\mathbf{u}^{h}}{\partial t}\right|_{h}|\mathbf{U}^{+}-\mathbf{U}^{-}|_{h}+\frac{1}{\Delta t}|\mathbf{U}^{+}-\mathbf{U}^{-}|_{h}^{2}. \tag{4.22}$$

With the aid of (4.19) it follows that

$$I_{2}\leqslant C|\mathbf{E}|_{h}^{2}+C|\mathbf{U}^{+}-\mathbf{U}^{-}|_{h}^{2}. \tag{4.23}$$

We split the third term via

$$\begin{aligned}I_{3}&=\left(|\mathbf{u}^{h}|^{\rho}A\mathbf{u}^{h}-|\mathbf{U}^{-}|^{\rho}A\mathbf{U}^{-},\mathbf{E}^{+}\right)^{h}+\left(|\mathbf{U}^{-}|^{\rho}A\mathbf{U}^{-}-|\mathbf{U}^{-}|^{\rho}A\mathbf{U}^{+},\mathbf{E}^{+}\right)^{h}\\&\equiv I_{3,1}+I_{3,2}.\end{aligned} \tag{4.24}$$

It follows from (2.6), a generalised Hölder inequality for S^h (cf. (3.6)), assumption (A3), Lemmata 3.2, 3.5 and 4.2, the Young's inequality (2.11) with $\varepsilon = 4$, and (4.19) that

$$I_{3,1} \leqslant \int_\Omega \pi^h\{||\mathbf{u}^h|^\rho A\mathbf{u}^h - |\mathbf{U}^-|^\rho A\mathbf{U}^-||\mathbf{E}^+|\}\,dx \leqslant C|\mathbf{E}|_h^2 + C|\mathbf{U}^+ - \mathbf{U}^-|_h^2 + \frac{1}{4}|\mathbf{E}^+|_1^2. \quad (4.25)$$

Noting (2.2*b*), a generalised Hölder inequality for S^h (cf. (3.6)), assumption (A3), Lemmata 3.2 and 4.2, the Young's inequality (2.11) with $\varepsilon = 4$, and (4.19) yield

$$I_{3,2} \leqslant \sqrt{\lambda_1^2 + \omega_1^2}\int_\Omega \pi^h\{|\mathbf{U}^-|^\rho|\mathbf{U}^+ - \mathbf{U}^-||\mathbf{E}^+|\}\,dx \leqslant C|\mathbf{E}|_h^2 + C|\mathbf{U}^+ - \mathbf{U}^-|_h^2 + \frac{1}{4}|\mathbf{E}^+|_1^2. \quad (4.26)$$

From (4.21)–(4.26) and a kickback of $\frac{1}{2}|\mathbf{E}^+|_1^2$ we have

$$\frac{d}{dt}|\mathbf{E}|_h^2 + |\mathbf{E}^+|_1^2 \leqslant C|\mathbf{E}|_h^2 + C\left|\frac{\partial \mathbf{u}^h}{\partial t}\right|_h |\mathbf{U}^+ - \mathbf{U}^-|_h + \frac{C}{\Delta t}|\mathbf{U}^+ - \mathbf{U}^-|_h^2. \quad (4.27)$$

Using the Grönwall lemma and recalling that $\mathbf{E}(0) = 0$ yield, for a.e. $t \in (0, T)$,

$$|\mathbf{E}(t)|_h^2 + \int_0^t |\mathbf{E}^+(s)|_1^2\,ds \leqslant C\exp(Ct)\int_0^t \left\{\left|\frac{\partial \mathbf{u}^h(s)}{\partial t}\right|_h |\mathbf{U}^+(s) - \mathbf{U}^-(s)|_h + \frac{1}{\Delta t}|\mathbf{U}^+(s) - \mathbf{U}^-(s)|_h^2\right\} ds \leqslant C\Delta t, \quad (4.28)$$

after noting the Cauchy–Schwarz inequality and Lemmata 3.5 and 4.2. With the bound (4.5) it is easy to show that $\|\mathbf{E} - \mathbf{E}^+\|^2_{L^\infty(0,T;L^2(\Omega))} \leqslant C\Delta t$, and thus

$$\|\mathbf{E}^+\|^2_{L^\infty(0,T;L^2(\Omega))} \leqslant 2\|\mathbf{E}^+ - \mathbf{E}\|^2_{L^\infty(0,T;L^2(\Omega))} + 2\|\mathbf{E}\|^2_{L^\infty(0,T;L^2(\Omega))} \leqslant C\Delta t,$$

hence $\|\mathbf{E}^+\|^2_{L^\infty(0,T;L^2(\Omega))} + \|\mathbf{E}^+\|^2_{L^2(0,T;H^1(\Omega))} \leqslant C\Delta t$. After recalling the semi-discrete error bound (Lemma 3.6) and the splitting $\mathbf{u} - \mathbf{U}^+ \equiv \mathbf{e} + \mathbf{E}^+$ we obtain (4.17). □

Remark In the proof of the fully discrete error bound we used an approach for piecewise-linear finite element approximations applied previously to a fourth-order nonlinear degenerate parabolic problem [7] and Cahn–Hilliard equations [2, 4, 5].

5 Numerical experiments

After recalling an analytical solution on the real line we discuss the numerical calculation of norms in 1-D. Programs for the 1-D experiments were written in FORTRAN 77, while MATLAB (version 6.5.1 - R13) was used for the 2-D experiments.

5.1 Preliminaries

The λ–ω system with $\rho = 2$ has on the real line a unique one-parameter family of periodic plane wave solutions given by

$$\begin{matrix} u(x,t) \\ v(x,t) \end{matrix} = \widehat{r} \begin{matrix} \cos \\ \sin \end{matrix} \left\{ \omega(\widehat{r})t + [\lambda(\widehat{r})]^{1/2} x \right\}, \tag{5.1}$$

where $\widehat{r}$ is the constant amplitude [26]. A necessary condition for the λ–ω system to possess periodic plane waves is $\widehat{r} < r_{\max} := \left(\frac{\lambda_0}{\lambda_1}\right)^{1/2}$. From a result in Kopell & Howard [26] (equation (41), p.317), it follows that the travelling-wave solutions of the λ–ω system are linearly stable if and only if $\widehat{r} \geqslant r_{\min} := \sqrt{\frac{2\lambda_0(\omega_1^2+\lambda_1^2)}{\lambda_1(2\omega_1^2+3\lambda_1^2)}}$. Thus, the condition $r_{\min} \leqslant \widehat{r} < r_{\max}$ provides a practical range of values for the amplitude to choose from in our calculations.

For the purpose of numerically verifying the fully discrete error bound in 1-D, note that the norms in space can be evaluated exactly, since for all $v^h \in S^h$

$$\|v^h\|_0^2 = \frac{h}{3}\sum_{j=0}^{J-1}\left[(v_{j+1}^h)^2 + v_{j+1}^h v_j^h + (v_j^h)^2\right], \quad |v^h|_1^2 = \frac{1}{h}\sum_{j=0}^{J-1}(v_{j+1}^h - v_j^h)^2,$$

where $v_j^h \equiv v^h(x_j)$, $v_{j+1}^h \equiv v^h(x_{j+1})$.

Recall the definition of $\mathbf{U}^+(t)$ in §4 (equation (4.18)). We make a similar definition corresponding to the exact solution $\mathbf{u}$ via $\mathbf{u}^+(t) := \pi^h \mathbf{u}(t_n)$, $\quad t \in (t_{n-1}, t_n]$, $n \geqslant 1$, i.e. we take the piecewise-linear interpolant of the exact solution in space and extend this solution in time using the piecewise-constant interpolant. We numerically verify the following version of the fully-discrete error bound (4.17) in 1-D, which follows as the exact solution (5.1) is in $C^\infty(\Omega_T)$ (for a proof see Garvie [20, Proposition 6.1.1]):

$$\|\mathbf{u}^+ - \mathbf{U}^+\|_{L^\infty(0,T;L^2(\Omega))} + \|\mathbf{u}^+ - \mathbf{U}^+\|_{L^2(0,T;H^1(\Omega))} \leqslant C(\Delta t^{1/2} + h), \tag{5.2}$$

where $\mathbf{u}$ corresponds to the analytical solution (5.1). Given an analytical solution we can calculate exactly the left hand side of the error bound (5.2) (for the component u) via the quantities

$$\xi_0(h, \Delta t) := \|u^+ - U^+\|_{L^2(0,T;H^1(\Omega))}^2 = \Delta t \sum_{n=1}^{N}\left[\|\pi^h u(t_n) - U^n\|_0^2 + |\pi^h u(t_n) - U^n|_1^2\right], \tag{5.3}$$

$$\xi_\infty(h, \Delta t) := \|u^+ - U^+\|_{L^\infty(0,T;L^2(\Omega))}^2 \equiv \max_{1\leqslant n \leqslant N} \|\pi^h u(t_n) - U^n\|_0^2. \tag{5.4}$$

The analytical solution (5.1) is given on the unbounded domain $\mathbb{R}$, thus, to make comparisons with the approximate solution on $\Omega = (0, L)$, we use time-dependent Neumann boundary conditions for our numerical method corresponding to the analytical solution (see next subsection). Provided the 'regularity' of the semi-discrete and fully discrete solutions are sufficient to control the boundary terms on the right-hand side of the corresponding weak formulations, then the error bound (4.17) will still apply. Numerous numerical experiments in 1-D indicate that if we are sufficiently far from the boundary to avoid 'pollution' of the solution obtained with homogeneous Neumann boundary conditions, then there is good qualitative agreement with the approximations using time-dependent Neumann boundary conditions.

5.2 Practical algorithms

We implement the following fully discrete, semi-implicit in time, finite element approximation, which is the complex equivalent of $(\mathrm{P}_1^{h,\Delta t})$ (see (4.3)), but with Neumann boundary data corresponding to (5.1):

$(\mathbf{P}_2^{h,\Delta t})$ For $n = 1,\ldots,N$ find $C^n \in \mathbb{S}^h$ such that $C^0 := P^h c_0$ and

$$\left(\frac{C^n - C^{n-1}}{\Delta t}, \chi^h\right)^h + (\nabla C^n, \nabla \chi^h) = \left(\widehat{f}(C^{n-1})C^n, \chi^h\right)^h + c_x(L,t)\chi^h(x_J) - c_x(0,t)\chi^h(x_0), \quad \forall \chi^h \in \mathbb{S}^h$$
$$\text{where} \quad \widehat{f}(C) := \lambda(R) + i\omega(R), \quad R \equiv |C|, \quad C := U + iV,$$

and from the Neumann boundary data we have

$$c_x(0,t) := u_x(0,t) + i\,v_x(0,t) = i\,\widehat{r}[\lambda(\widehat{r})]^{1/2} \exp\{i\,\omega(\widehat{r})t\},$$
$$c_x(L,t) := u_x(L,t) + i\,v_x(L,t) = i\,\widehat{r}[\lambda(\widehat{r})]^{1/2} \exp\left\{i\,\left(\omega(\widehat{r})t + [\lambda(\widehat{r})]^{1/2}L\right)\right\}.$$

Choosing $C^n = \sum_{j=0}^{J} C_j^n \varphi_j$, $\chi^h = \varphi_i$, $i = 0,\ldots,J$ where $C_j^n \approx c(jh, n\Delta t)$ leads to the following tri-diagonal system of $(J+1)$ linear equations, with complex coefficients:

$$A_{n-1}\mathbf{C}^n = \mathbf{C}^{n-1} + \mathbf{b}(t), \quad \mathbf{C}^0 := M^{-1}\mathbf{C}_0, \tag{5.5}$$
$$\text{where} \quad A_{n-1} := I - \Delta t\,\mathrm{diag}\{\widehat{f}(C_0^{n-1}),\ldots,\widehat{f}(C_J^{n-1})\} + \Delta t(\widehat{M})^{-1}K,$$
$$\mathbf{C}^n := (C_0^n,\ldots,C_J^n)^T, \quad C_j^n := U_j^n + i\,V_j^n, \quad R_j^n \equiv |C_j^n|, \quad \{\mathbf{C}_0\}_j := (c_0, \varphi_j),$$
$$\text{and} \quad \{\mathbf{b}(t)\}_j := \frac{2\Delta t}{h}\begin{cases} -c_x(0,t) & \text{for } j = 0, \\ 0 & \text{for } 1 \leqslant j \leqslant J-1, \\ c_x(L,t) & \text{for } j = J, \end{cases}$$

(recall (3.1), (3.2)). We chose the initial approximations to correspond to the interpolant of the analytical solutions at $t = 0$.

5.3 Results in 1-D

Results for $(\mathrm{P}_2^{h,\Delta t})$ are presented on a uniform partition of $\Omega = (0,L)$, for $0 \leqslant t \leqslant T$, with mesh points $x_j = jh$, $j = 0,\ldots,J$, where $h := L/J$. The system (5.5) was solved directly and, for Δt sufficiently small, is strictly diagonally dominant and thus no partial pivoting is required. To test the error bound we chose the following data: $L = 60$, $T = 1/6$, $\rho = 2$, $\lambda_0 = 3$, $\lambda_1 = 2$, $\omega_0 = -5$, $\omega_1 = 1$. The amplitude was set at $\widehat{r} = (r_{\max} + r_{\min})/2 \approx 1.1299$.

Table 1. *Numerical results from* ($P_2^{h,\Delta t}$) *used to test the error bound in Theorem 4.1.* $\Delta t = 1/80$ *and the space step is successively halved*

h	$\xi_0(h, 1/80)$	$\xi_\infty(h, 1/80)$	R_0^h (3 s.f.)	R_∞^h (3 s.f.)
1/2	0.0198878034	0.0891816059	3.92	3.92
1/4	0.020155689	0.0909897348	3.91	3.89
1/8	0.0202240452	0.0914510397	4.00	3.81
1/16	0.020241534	0.0915695369	–	–
1/32	0.0202459105	0.0916006106	–	–

Table 2. *Numerical results from* ($P_2^{h,\Delta t}$) *used to test the error bound in Theorem 4.1.* $h = 1/4$ *and the time step is successively halved*

Δt	$\xi_0(1/4, \Delta t)$	$\xi_\infty(1/4, \Delta t)$	$R_0^{\Delta t}$ (3 s.f.)	$R_\infty^{\Delta t}$ (3 s.f.)
1/80	0.0201556965	0.0909897574	3.74	3.92
1/160	0.00527169516	0.0230973836	4.12	4.01
1/320	0.0012926067	0.00575748705	3.95	4.01
1/640	0.000325840155	0.00143159815	–	–
1/1280	8.08132988E-05	0.000352038359	–	–

We computed the ratios (see (5.3), (5.4))

$$R_i^h := \frac{\xi_i(h, \Delta t) - \xi_i(h/2, \Delta t)}{\xi_i(h/2, \Delta t) - \xi_i(h/4, \Delta t)}, \quad R_i^{\Delta t} := \frac{\xi_i(h, \Delta t) - \xi_i(h, \Delta t/2)}{\xi_i(h, \Delta t/2) - \xi_i(h, \Delta t/4)}, \quad i = 0, \infty \tag{5.6}$$

which led to the results in Tables 1 and 2 for discretisation in space and time, respectively. Assuming the quantities $\xi_0(h, \Delta t)$, $\xi_\infty(h, \Delta t)$ can be written as $ah^p + A(\Delta t)^q$, $p, q \in \mathbb{N}$, $a, A \in \mathbb{R}$, then $R_i^h = 2^p$ and $R_i^{\Delta t} = 2^q$ $(i = 0, \infty)$. From the tabulated results we conclude $p = q = 2$, $|a| \ll |A|$, and so it may be possible to improve the theoretical result that the error bound is of order 1/2 in the time step. Furthermore, the condition $|a| \ll |A|$ implies that the contribution to the error from space discretisation is much less than the contribution to the error from time discretisation. Thus it is possible to have $\frac{\xi_i(h,\Delta t)}{\xi_i(h/2,\Delta t)} \approx 1$, $(i = 0, \infty)$, when Δt is much smaller than h. This is reflected in our observation that provided the space step is small compared to the wavelength of the travelling-wave solutions, then the basic qualitative features of the solution are independent of refinements of the mesh in space.

In Figures 1(a)–(d), the numerical solution U^n of ($P_2^{h,\Delta t}$) and the exact solution $u(x, t)$ of (5.1) are plotted together at time intervals of 5 units, where $L = 60$ and $T = 20$. In these experiments we reduce Δt with h fixed at 1/8. As Δt is increased above the critical value of $1/[\lambda_0(2\rho + 2)] = 1/18$ (see Lemma 4.2) the amplitude reduces to zero, corresponding to a stable fixed point at (0,0) of the numerical scheme. As the origin in the u-v plane is an unstable fixed point of the linearised λ–ω system this behaviour illustrates a spurious solution of the numerical scheme for large Δt. At the critical value of $\Delta t = 1/18$ the amplitude of the numerical solution matches the amplitude of the exact solution well,

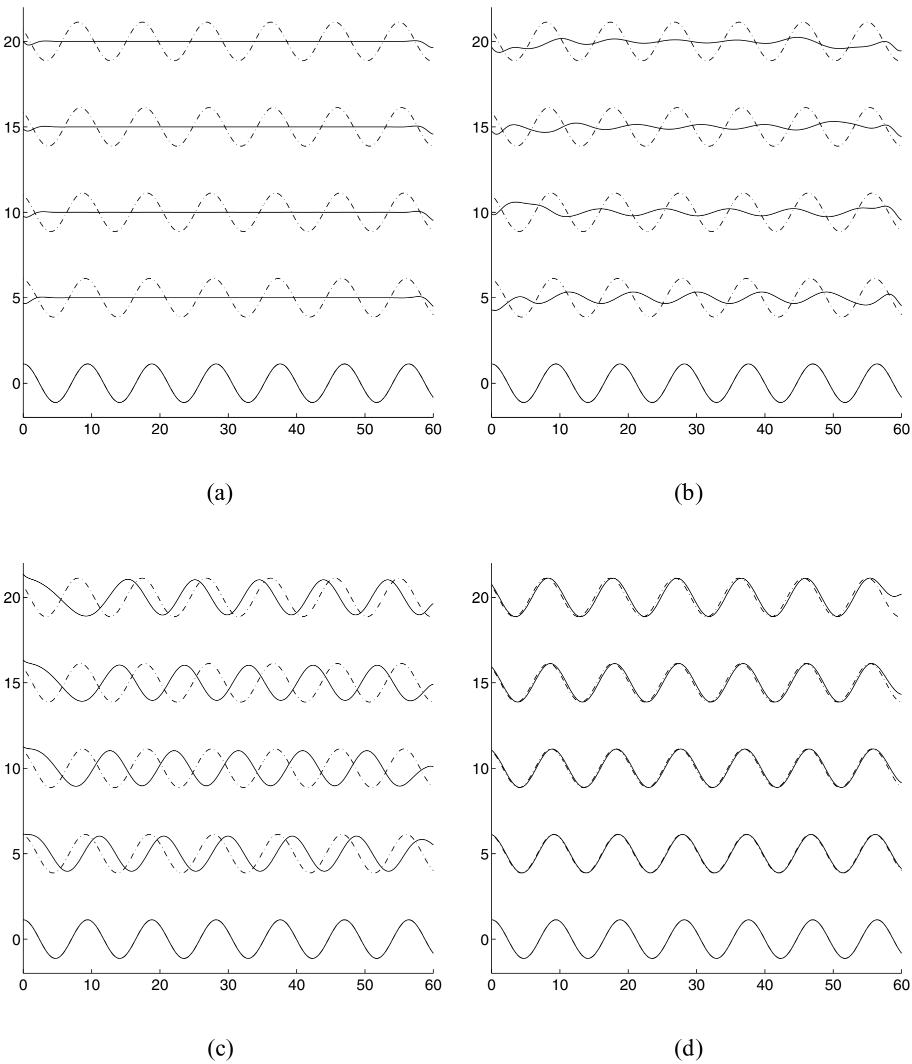

FIGURE 1. (a)–(d) Typical numerical solutions U^n, denoted —— and exact solution $u(x, t)$, denoted $\cdot - \cdot -$ of the $\lambda - \omega$ system are plotted as a function of space x at times $t = 0, 5, 10, 15, 20$ with the following parameter values: $\rho = 2$, $\lambda_0 = 3$, $\lambda_1 = 2$, $\omega_0 = -5$, $\omega_1 = 1$, $\widehat{r} \approx 1.1299$. Plots show successive refinement of Δt with h fixed at 1/8: (a) $\Delta t = 1/3$, (b) $\Delta t = 1/6$, (c) $\Delta t = 1/18$, (d) $\Delta t = 1/320$. The initial approximations are given by $U^0 = \pi^h u(x, 0)$.

but the phase is poorly reproduced. As Δt is reduced below 1/18 the poorly represented phase recovers until at $\Delta t = 1/320$ there is good qualitative agreement between the approximate and the exact solution, except at $x = L$. An explanation for this may be the following. If we express the exact solution in the form $u(x, t) = \alpha \cos \beta(x - ct)$ then we have $c = -\omega(\widehat{r})/\sqrt{\lambda(\widehat{r})} \approx 5.57$, i.e. the speed of the travelling waves is positive, resulting in the propagation of errors to the right-hand side of the domain. The discrepancy between the exact and approximate solutions at $x = L$ disappears as Δt is further reduced.

5.4 Results in 2-D

Numerical results for the complex equivalent of the finite element scheme ($\mathrm{P}_1^{h,\Delta t}$) (scheme ($\mathrm{P}_2^{h,\Delta t}$) with zero boundary data) are presented in two dimensions on a uniform mesh constructed from the 'right-angled' triangulation of the square $\Omega = (-L, L) \times (-L, L)$. We used the natural ordering of the nodes $(ih - L, jh - L)$, where $i, j = 0, \ldots, \sqrt{J+1} - 1$. In all experiments we took $h = 1/4$, $\Delta t = 1/384$, and $L = 50$. The resulting linear system, namely (5.5) with $\mathbf{b} \equiv \mathbf{0}$, was solved at each time step using the GMRES algorithm in MATLAB, with a restart value of 4, and default settings for the tolerance (of the relative error) and the maximum number of total iterations. At each time step the solution at the previous time level was used as the initial guess for the iterative solver. For further details concerning MATLAB's GMRES algorithm see the description in the help pages for MATLAB.

Figures 2(a), (c) and (e) show approximations of V^n at times $T = 10$, 20, and 30 respectively, evolving from Gaussian initial data at the origin, namely $U^0 = V^0 = \pi^h 0.1 \exp\{-0.8(x^2 + y^2)\}$. The parameter values used were: $\lambda_0 = 1/2$, $\lambda_1 = 1/10$, $\omega_0 = -1/10$, $\omega_1 = 1$, and $\rho = 3/2$. The resulting 'target waves' are known to exist as solutions to reaction-diffusion systems of λ–ω type [21, 27].

Figures 2(b), (d) and (f) show approximations of U^n at times $T = 5$, 15, and 75, respectively, evolving from the perfect Archimedian spiral wave $C^0 = \pi^h R \exp\{i(\theta + R/2)\}/35$, $C^0 = U^0 + iV^0$, where (R, θ) are polar coordinates. The parameter values used were $\lambda_0 = 1$, $\lambda_1 = 1$, $\omega_0 = 3$, $\omega_1 = -3$, and $\rho = 2$. The initially perfect rotating spiral wave starts to break up around $T = 15$, and at $T = 75$ has evolved into irregular patchy structures ('turbulence') covering the whole domain. Spiral waves have been proved to exist as solutions of systems [15], and numerous authors have investigated spiral solutions of λ–ω systems [17, 22, 23, 25, 29]. The phenomenon of spiral break-up has also been investigated [12, 28, 29].

6 Summary and discussion

We proved an error bound for a fully practical piecewise-linear finite element approximation, using a semi-implicit time discretisation of a nonlinear reaction-diffusion system of λ–ω type. The fully discrete error bound was proved to be of order 1/2 in the time step and first order in the space step. All results cover the important case when $\rho = 2$ in one and two dimensions. The complex numerical method is fully practical in the sense that it is easy to implement on a computer and there are no prohibitive conditions on the mesh parameters and time step. The fully discrete error bound was verified numerically with the aid of an explicit solution in 1-D. Results indicate that the error bound is first order in the time step, and that errors due to refinements of the space step are much less than errors resulting from time discretisation (at least in 1-D). Experiments in 2-D led to the three basic types of spatiotemporal dynamics reported in the literature for λ–ω systems, namely, 'target patterns', spiral waves, and 'turbulence'.

Our methodology was to mimic the continuous estimates in Part I of this work [11]. This led us to extend the theoretical framework of the finite-dimensional space S^h by

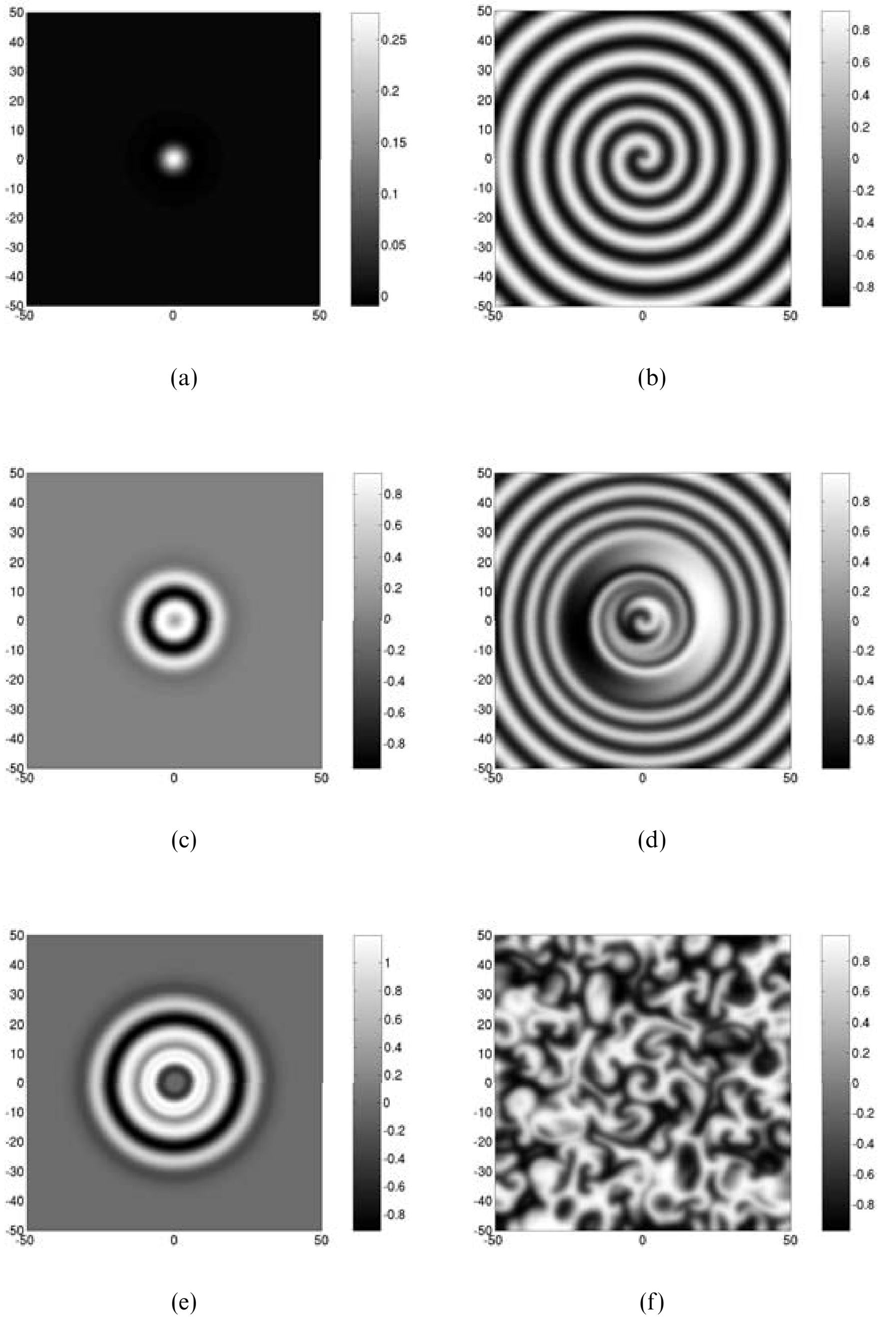

FIGURE 2. Snapshots of approximate target patterns for V^n at (a) $T = 10$, (c) $T = 20$, (e) $T = 30$, and snapshots of approximate spiral wave 'break-up' for U^n at (b) $T = 5$, (d) $T = 15$, (f) $T = 75$. In all plots $h = 1/4$ and $\Delta t = 1/384$. See text for initial data and parameter values.

constructing new mesh-dependent norms and proving associated results, which may be useful to other researchers studying the numerics of nonlinear PDEs.

The numerical analysis of the λ–ω system in this work is applicable to systems of reaction-diffusion equations with reaction kinetics close to a supercritical Hopf bifurcation. Furthermore, the overall approach and techniques developed in this paper are applicable to general reaction-diffusion systems, thus it would be natural to try and use the methods in this work to undertake the analysis of more realistic problems, for example, in ecology or epidemiology.

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