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Finite element approximation of spatially extended predator–prey interactions with the Holling type II functional response

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Abstract We study the numerical approximation of the solutions of a class of nonlinear reaction–diffusion systems modelling predator–prey interactions, where the local growth of prey is logistic and the predator displays the Holling type II functional response. The fully discrete scheme results from a finite element discretisation in space (with lumped mass) and a semi-implicit discretisation in time. We establish a priori estimates and error bounds for the semi discrete and fully discrete finite element approximations. Numerical results illustrating the theoretical results and spatiotemporal phenomena are presented in one and two space dimensions. The class of problems studied in this paper are real experimental systems where the parameters are associated with real kinetics, expressed in nondimensional form. The theoretical techniques were adapted from a previous study of an idealised reaction–diffusion system (Garvie and Blowey in Eur J Appl Math 16(5):621–646, 2005).

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1 Introduction

Let Ω be a bounded domain in $\mathbb{R}^d$, $d \leq 3$, with Lipschitz boundary $\partial\Omega$. We study the following nondimensional system modelling predator–prey interactions:

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Find the prey $u(\mathbf{x}, t)$ and predator $v(\mathbf{x}, t)$ densities such that

$$\frac{\partial u}{\partial t} = \Delta u + u(1-u) - v\,h(au) \quad \text{in } \Omega_T := \Omega \times (0, T), \tag{1.1a}$$

$$\frac{\partial v}{\partial t} = \delta \Delta v + b\,v\,h(au) - c\,v \quad \text{in } \Omega_T, \tag{1.1b}$$

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

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

where $\boldsymbol{\nu}$ denotes the outward normal to $\partial\Omega$, and $\Delta = \sum_{i=1}^{d} \partial^2/\partial x_i^2$. The parameters a, b, c, and δ are real and strictly positive, and the functional response $h(\cdot)$ represents the instantaneous, per capita, feeding rate, as a function of prey abundance. Note that the local growth of the prey is logistic and the predator shows the 'Holling type II functional response' [26]. For details of the nondimensionalisation procedure see Garvie MR and Trenchea C (Analysis of two generic spatially extended predator–prey models. Nonlinear Anal. Real World Appl., submitted).

We consider the following well-known (nondimensional) type II functional responses with positive parameters α, β, and γ

$$h(\eta) = h_1(\eta) = \frac{\eta}{1+\eta} \quad (\eta = au), \text{ with } a = 1/\alpha, b = \beta, c = \gamma, \tag{1.2a}$$

$$h(\eta) = h_2(\eta) = 1 - e^{-\eta} \quad (\eta = au), \text{ with } a = \gamma, c = \beta, b = \alpha\beta, \tag{1.2b}$$

due originally to Holling [27] and Ivlev [32], respectively. Thus the two types of kinetics considered in this paper are given by:

Kinetics (i) :

$$f(u, v) = u(1-u) - \frac{uv}{u+\alpha}, \quad g(u, v) = \frac{\beta uv}{u+\alpha} - \gamma v,$$

Kinetics (ii) :

$$f(u, v) = u(1-u) - v\left(1 - e^{-\gamma u}\right), \quad g(u, v) = \beta v\left(\alpha - 1 - \alpha e^{-\gamma u}\right).$$

We focus on dynamics in the positive quadrant $u \geq 0, v \geq 0$, corresponding to biologically meaningful solutions. From linear stability analysis one finds that in both cases we have saddle points at $(0, 0)$ and $(1, 0)$. There is also a stationary point (u^*, v^*) (stable or unstable) corresponding to the coexistence of prey and predators given by

$$u^* = \frac{\alpha\gamma}{\beta - \gamma}, \quad v^* = (1-u^*)(u^* + \alpha), \;\; \beta > \gamma, \;\; \alpha < \frac{\beta - \gamma}{\gamma}, \tag{1.3a}$$

$$u^* = -\frac{1}{\gamma} \ln\left(\frac{\alpha - 1}{\alpha}\right), \quad v^* = \frac{u^*(1-u^*)}{1 - e^{-\gamma u^*}}, \;\; \alpha > 1, \;\; \gamma > -\ln\left(\frac{\alpha - 1}{\alpha}\right), \tag{1.3b}$$

for Kinetics (i) and (ii), respectively. The restrictions on the parameters (assumed throughout) follow from the necessary condition $0 < u^* < 1$, which is readily obtained from a consideration of the nullclines (the solution curves corresponding to the equations $f = 0$ and $g = 0$). For appropriate choices of the parameters, the kinetics have a stable limit cycle surrounding the unstable stationary point (u^*, v^*), i.e., the densities of predators and prey cycle periodically in time. In both cases $b > c$, which plays a small part in later estimates. Naturally we are only interested in nonnegative solutions of the full PDE system, and the appropriate choice of initial data will guarantee this (see discussion below). The advantage of expressing the reaction–diffusion system in the form (1.1a)–(1.1b) is that our analysis covers Kinetics (i) and (ii) simultaneously.

We give some brief background details about the systems studied, before discussing our goals in this paper. Type II functional responses are the most frequently studied functional responses, and are well-documented in empirical studies (for review papers see [20,33,57]). When the functional response is of type II, the predation rate approaches an asymptote along a saturating curve (inverse density dependence). For ecological and modelling details and explicit forms of the various functional responses (type I, II and III) see [6,22,34,37].

The system of ordinary differential equations (ODEs), i.e., the spatially homogeneous system corresponding to (1.1a)–(1.1b) with the functional responses $h_1(\cdot)$ or $h_2(\cdot)$, has been well-studied [16,36,42]. The ODE system corresponding to Kinetics (i) is sometimes called the Rosenzweig–MacArthur model [52], and has been used in many studies to fit ecological data. However, there are few papers concerning the ('spatially extended') reaction–diffusion system, which takes into account both spatial and temporal dynamics of predators and prey. For an introduction to this area see [28] and the references therein.

A work that partly motivated our study is a SIAM Review paper [38] that considers the reaction–diffusion system (1.1a)–(1.2a) as a model for marine plankton dynamics. The paper [38] has an extensive reference list, and for various initial conditions the authors show numerically that the evolution of the system leads to the formation of spiral patterns, followed by irregular patches spreading over the whole domain (spatiotemporal chaos), which are in qualitative agreement with field observations. For additional recent studies of the reaction–diffusion systems considered in our paper, see the papers by Petrovskii and Malchow [35,46–48], the papers by Sherratt et al. [54–56], and also [3,21,49,53]. There is also a large body of related work by the Japanese school of researchers in reaction–diffusion equations. For example, Mimura et al. have studied: cross-diffusion competition systems [29,40], dynamics of models for chemotaxis growth [2,7,17], pattern formation in resource–consumer systems [15,39], asymptotic analysis of interface dynamics for competition–diffusion models [10–12], interaction of travelling pulse solutions [13,31,41], interface dynamics for two-phase Stefan like problems [23–25], and travelling waves in bistable reaction–diffusion systems [30,31,43].

It is the goal of this paper to develop a fully discrete finite element approximation that is easy to implement, with known stability and accuracy properties. Our hope is that applied mathematicians will find the numerical method useful as a starting point for investigating the key dynamical properties of spatially extended predator–prey interactions. The use of algorithms with known stability and accuracy properties is particularly important for the systems studied in this paper due to the inherent chaotic nature of the solutions [56]. When interpreting numerical results it is important to be able to distinguish between the onset of numerical instability, and chaos that is a true feature of the underlying continuous model.

The theoretical techniques in this paper were adapted from the study of an idealised reaction–diffusion system [19], which possesses a simple energy property that is readily mimicked in the discrete case. For the systems studied in this paper the situation is more complicated. Even in the continuous case, without some knowledge of the positivity of solutions the basic estimates fail. Fortunately, provided we choose bounded, nonnegative initial data, the continuous solutions remain nonnegative on their intervals of existence [58, Lemma 14.20]. Thus the usual a priori estimates can be derived. However, in the discrete case the lack of a practical discrete maximum principle (see Thomée [59]) means we cannot guarantee that approximations remain nonnegative. As a consequence the discrete kinetic functions cease to be locally Lipschitz continuous, driving possible blow-up in finite time. In order to mimic the estimates in the continuous case and circumvent these problems, we modify the logistic growth term and the functional responses by taking the modulus of appropriate u terms, which leads to some technical complications in the semi discrete error analysis (see Sect. 2).

We are not aware of any numerical analysis of these systems. The paper is structured in the following way. In Sect. 2 we undertake a rigorous numerical analysis of the predator–prey systems using a semi discrete, piecewise linear, finite element method, leading to a priori estimates and a semi discrete error bound. In Sect. 3 we formulate a fully discrete finite element method, and provide stability estimates and a fully discrete error bound. In Sect. 4 we provide some implementational details, numerically verify the error bound in one space dimension, and provide some numerical computations in one and two space dimensions. We make some conclusions in Sect. 5.

Notation and mathematical preliminaries

Let X and Y be Banach spaces where $X \hookrightarrow Y$ denotes that X has continuous injection into Y, and the dual space of X is written X'. We have adopted the standard notation for the Sobolev spaces $W^{m,p}(\Omega)$, $m \in \mathbb{N}$, $p \in [1, \infty]$, with associated norms and semi-norms given by $\|u\|_{m,p}$ and $|u|_{m,p}$. D^{α} is the standard multi-index notation for the mixed (generalised) partial derivatives of order $|\alpha|$ ($\alpha_i \in \mathbb{N} \cup \{0\}$). When $p = 2$, $W^{m,2}(\Omega)$ is denoted $H^m(\Omega)$ with norm $\|\cdot\|_m$ and semi-norm $|\cdot|_m$, and if additionally $m = 0$, $W^{0,2}(\Omega) \equiv L^2(\Omega)$. The usual L^2 inner product over Ω with norm $\|\cdot\|_0$ is denoted by $(\cdot, \cdot)$. A norm on $(H^m(\Omega))'$, $m > 0$, is given by

$$\|f\|_{-m} := \sup_{0 \neq v \in H^m(\Omega)} \frac{\langle f, v \rangle}{\|v\|_m}, \quad \forall f \in (H^m(\Omega))',$$

where $\langle f, v \rangle$ represents the duality pairing between $(H^m(\Omega))'$ and $H^m(\Omega)$. Spaces consisting of vector-valued functions are denoted in bold face, e.g., $\mathbf{H}^1(\Omega) = (H^1(\Omega))^2$. In Sect. 2 we need norms and semi-norms defined on a single reference simplex τ, which we represent via $\|\cdot\|_{m,p,\tau}$ and $|\cdot|_{m,p,\tau}$ (or $\|\cdot\|_{m,\tau}$ and $|\cdot|_{m,\tau}$ if $p=2$), respectively.

We shall need the following simple versions of the Sobolev Embedding Theorem (e.g., [8, p. 114])

$$H^1(\Omega) \hookrightarrow L^q(\Omega) \quad \text{for} \quad q \in \begin{cases} [1,\infty] & \text{if } d=1, \\ [1,\infty) & \text{if } d=2, \\ [1,6] & \text{if } d=3, \end{cases} \tag{1.4}$$

$$H^{\frac{d}{2}+\varepsilon}(\Omega) \hookrightarrow C(\bar{\Omega}), \quad \varepsilon > 0, \tag{1.5}$$

and a Sobolev interpolation result (e.g., see [1]): let $s \in [1,\infty]$, $m \geq 1$ 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

$$\|v\|_{0,r} \leq C\|v\|_{0,s}^{1-\mu}\|v\|_{m,s}^{\mu} \quad \text{for } r \in \begin{cases} [s,\infty] & \text{if } m - \frac{d}{s} > 0, \\ [s,\infty) & \text{if } m - \frac{d}{s} = 0, \\ [s, -\frac{d}{m-(d/s)}] & \text{if } m - \frac{d}{s} < 0. \end{cases} \tag{1.6}$$

For later purposes we recall the following Grönwall lemma in differential form: 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 nonnegative. Then,

$$\frac{dE}{ds} + P(s) \leq R(s)E(s) + Q(s) \quad \text{a.e. in } [0,t], \tag{1.7}$$

implies

$$E(t) + \int_0^t P(\tau)\,d\tau \leq e^{\Lambda(t)}E(0) + e^{\Lambda(t)}\int_0^t Q(\tau)\,d\tau, \tag{1.8}$$

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

In order to obtain a fully discrete estimate we need the following monotonicity property: let $\mathbf{v}_1, \mathbf{v}_2 \in \mathbb{R}^n$, $n \in \mathbb{N}$, $p \geq 0$, then

$$|\mathbf{v}_1|^p\mathbf{v}_1 \cdot (\mathbf{v}_1 - \mathbf{v}_2) \geq \frac{|\mathbf{v}_1|^{p+2} - |\mathbf{v}_2|^{p+2}}{p+2}. \tag{1.9}$$

We recall a Young's inequality that holds for any $\varepsilon > 0$, $a, b \geq 0$, and $m, n > 1$:

$$ab \leq \varepsilon^{m/n}\frac{a^m}{m} + \frac{1}{\varepsilon}\frac{b^n}{n}, \qquad \frac{1}{m} + \frac{1}{n} = 1. \tag{1.10}$$

Another useful inequality, valid for arbitrary $a, b \geq 0$, $p > 0$, is [51]

$$2^{-(p-1)^-}(a^p + b^p) \leq (a+b)^p \leq 2^{(p-1)^+}(a^p + b^p), \tag{1.11}$$

where $q^{\pm} := \max\{\pm q, 0\}$. Throughout we let C denote a finite, positive constant, independent of the mesh and temporal discretisation parameters, possibly depending on T, Ω, u_0 and v_0.

The continuous problem

For notational convenience we express the predator–prey system (1.1a)–(1.1d) in the following vector form after taking $\mathbf{u} := (u, v)^T$:

$$\mathbf{u}_t = D\Delta\mathbf{u} + \mathbf{f}(\mathbf{u}), \quad \text{in } \Omega_T, \tag{1.12a}$$

$$\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), \quad \mathbf{x} \in \Omega, \qquad \frac{\partial \mathbf{u}}{\partial \boldsymbol{\nu}} = \mathbf{0} \quad \text{on } \partial\Omega \times (0, T), \tag{1.12b}$$

where

$$\mathbf{f}(\mathbf{u}) \equiv \begin{pmatrix} f(u, v) \\ g(u, v) \end{pmatrix} := \begin{pmatrix} u(1-u) - v\,h(au) \\ b\,v\,h(au) - c\,v \end{pmatrix}, \quad D := \begin{pmatrix} 1 & 0 \\ 0 & \delta \end{pmatrix}. \tag{1.12c}$$

The predator–prey system (1.12a)–(1.12c) leads to the introduction of the following weak formulation:

(**P**) Find $\mathbf{u}(\cdot, t) \in \mathbf{H}^1(\Omega)$ such that $\mathbf{u}(\cdot, 0) = \mathbf{u}_0(\cdot)$ and for a.e. $t \in (0, T)$

$$(\mathbf{u}_t, \boldsymbol{\eta}) + a_\delta(\mathbf{u}, \boldsymbol{\eta}) = (\mathbf{f}(\mathbf{u}), \boldsymbol{\eta}) \quad \forall \boldsymbol{\eta} \in \mathbf{H}^1(\Omega), \tag{1.13}$$

where $a_\delta(\cdot, \cdot)$ is a bilinear form given by

$$a_\delta(\mathbf{u}, \mathbf{v}) := (D\,\nabla\mathbf{u}, \nabla\mathbf{v}) \quad \forall \mathbf{u}, \mathbf{v} \in \mathbf{H}^1(\Omega), \tag{1.14}$$

with semi-norm

$$|\mathbf{u}|_{a_\delta} := \sqrt{|u|_1^2 + \delta |v|_1^2}, \tag{1.15}$$

equivalent to the $\mathbf{H}^1$ semi-norm, i.e.,

$$\sqrt{c_\delta}|\mathbf{u}|_1 \le |\mathbf{u}|_{a_\delta} \le \sqrt{C_\delta}|\mathbf{u}|_1, \quad c_\delta := \min\{1, \delta\}, \quad C_\delta := \max\{1, \delta\}. \tag{1.16}$$

Using results from semigroup theory and a Lyapunov function approach, Garvie MR and Trenchea C (Analysis of two generic spatially extended predator–prey models. Nonlinear Anal. Real World Appl., submitted) proved that the classical solutions of the predator–prey system are globally well-posed and nonnegative, given nonnegative, bounded initial data, with a domain of class $C^{2+\nu}$, $\nu > 0$. However for the application of the finite element method we assume for simplicity that the theoretical results in Garvie MR and Trenchea C (Analysis of two generic spatially extended predator–prey models. Nonlinear Anal. Real World Appl., submitted) also hold in the polygonal/polyhedral setting. More precisely, we assume the following result holds throughout this work: let Ω be a bounded domain in $\mathbb{R}^d$, $d \le 3$, with Lipschitz boundary $\partial\Omega$. Additionally, let $u_0, v_0 \in H^1(\Omega) \cap L^\infty(\Omega)$ be nonnegative initial data, then there exists a unique nonnegative strong solution $\{u, v\}$ of the predator–prey system (1.1a)–(1.1d) with functional response (1.2a) or (1.2b) such that

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

The requirement that $u_0, v_0 \in L^\infty(\Omega)$ is necessary for the proof of the global well-posedness of solutions as discussed above, while taking $u_0, v_0 \in H^1(\Omega)$ is a necessary requirement for the numerical analysis of the discrete problems.

2 Semi discrete approximations

Initially we discuss some results and assumptions associated with the finite element spaces. The main tools are given in [19], but for convenience the relevant results are summarised here. We consider the finite element approximation of (P) under the following assumptions on the mesh:

($\mathbf{A}^h$) Let $\Omega \subset \mathbb{R}^d$, $d \le 3$, be a polygonal domain if $d = 2$ and a polyhedral domain if $d = 3$. Let $\mathcal{T}^h$ be a quasi-uniform partitioning [8, p. 132] of Ω into disjoint open simplices $\{\tau\}$ with $h_\tau :=$ diam τ and $h := \max_{\tau \in \mathcal{T}^h} h_\tau$, so that $\overline{\Omega} = \cup_{\tau \in \mathcal{T}^h} \overline{\tau}$. Additionally, we assume $\mathcal{T}^h$ is weakly acute (e.g., [14], [44, 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 angles made by any two faces of the same tetrahedron does not exceed $\pi/2$.

Associated with $\mathcal{T}^h$ is the standard finite element space

$$S^h := \{v \in C(\overline{\Omega}) \ :\ v|_\tau \quad \text{is linear}\ \forall \tau \in \mathcal{T}^h\} \subset H^1(\Omega).$$

Let $\{\varphi_j\}_{j=0}^J$ be the standard basis for S^h, satisfying $\varphi_j(x_i) = \delta_{ij}$, where $\{x_i\}_{i=0}^J$ is the set of nodes of $\mathcal{T}^h$. We introduce $\pi^h : C(\overline{\Omega}) \mapsto S^h$, the Lagrange interpolation operator, such that $\pi^h v(x_j) = v(x_j)$ for all $j = 0, \ldots J$. A discrete L^2 inner product on $C(\overline{\Omega})$ is then defined by

$$(u, v)^h := \int_\Omega \pi^h(u(x)v(x))\, dx \equiv \sum_{j=0}^J \widehat{M}_{jj} u(x_j) v(x_j), \tag{2.17}$$

where $\widehat{M}_{jj} := (1, \varphi_j) \equiv (\varphi_j, \varphi_j)^h > 0$, corresponding to the (diagonal) lumped mass matrix $\widehat{M}$. We also define $K_{ij} := (\nabla\varphi_i, \nabla\varphi_j)$, corresponding to the stiffness matrix K.

We state some additional results concerning S^h. It is well-known that the discrete inner product (2.17) induces a norm on $S^h \subset C(\overline{\Omega})$ via

$$|\chi^h|_h := \sqrt{(\chi^h, \chi^h)^h} \quad \forall \chi^h \in S^h, \tag{2.18}$$

and the norms $\|\cdot\|_0$ and $|\cdot|_h$ are equivalent where the constants are independent of h [45,50]. The induced norm on S^h is generalised to the L^p setting for $1 \leq p < \infty$, by

$$|\chi^h|_{h,p} := \left(\int_\Omega \pi^h\{|\chi^h(x)|^p\}\,dx\right)^{1/p} \equiv \left(\sum_{j=0}^{J} \widehat{M}_{jj}|\chi^h(x_j)|^p\right)^{1/p}, \tag{2.19a}$$

and

$$|\chi^h|_{h,\infty} := \max_{0\leq j\leq J}|\chi^h(x_j)| \quad \text{if } p = \infty. \tag{2.19b}$$

We denote the Banach space $L^{h,p}(\Omega)$, $1 \leq p \leq \infty$, to be S^h equipped with the norm $|\cdot|_{h,p}$. The following results are easily verified for all $\chi^h, \psi^h \in S^h$:

$$|(\chi,\psi)^h| \leq |\chi|_{h,p}|\psi|_{h,q}, \quad \frac{1}{p}+\frac{1}{q} = 1, \quad 1 \leq p, q \leq \infty, \tag{2.20a}$$

$$|\chi^h|_{h,q} \leq C|\chi^h|_{h,p}, \quad C = |\Omega|^{1/q-1/p}, \quad 1 \leq q \leq p \leq \infty. \tag{2.20b}$$

A consequence of the weak acuteness property is that if $\mathbf{U}$ is a monotone function on $\mathbb{R}^n$, $n \in \mathbb{N}$, then [18, Lemma 4.2.1]

$$\left(\nabla\boldsymbol{\chi}^h, \nabla\pi^h\mathbf{U}(\boldsymbol{\chi}^h)\right) \geq 0 \quad \forall\boldsymbol{\chi}^h \in \{S^h\}^n. \tag{2.21}$$

We provide some results concerning a 'lumped' L^2 projection operator $Q^h : L^2(\Omega) \mapsto S^h$ satisfying

$$(Q^h\eta, \chi^h)^h = (\eta, \chi^h) \quad \forall\chi^h \in S^h.$$

It is easy to show that $Q^h\eta \equiv \sum_{j=0}^J \frac{(\eta,\varphi_j)}{(1,\varphi_j)}\varphi_j$ is well-defined, and that

$$\|Q^h\eta\|_{0,\infty} \equiv |Q^h\eta|_{h,\infty} \leq \|\eta\|_{0,\infty} \quad \forall\eta \in L^\infty(\Omega). \tag{2.22}$$

We also need the result [4,5]

$$\|(I-Q^h)\eta\|_0 + h|(I-Q^h)\eta|_1 \leq Ch|\eta|_1 \quad \forall\eta \in H^1(\Omega), \tag{2.23}$$

which leads to

$$\|Q^h\eta\|_1 \leq C\|\eta\|_1 \quad \forall\eta \in H^1(\Omega). \tag{2.24}$$

We also require the following well-known interpolation error estimates valid for $d \leq 3$ [9, Theorem 5]

$$\|(I-\pi^h)\chi\|_0 + h|(I-\pi^h)\chi|_1 \leq Ch^2|\chi|_2 \quad \forall\chi \in H^2(\Omega), \tag{2.25a}$$

$$\|(I-\pi^h)\chi\|_{0,1} \leq Ch^2|\chi|_{2,1} \quad \forall\chi \in W^{2,1}(\Omega), \tag{2.25b}$$

the inverse estimates [8, Theorem 3.2.6.]

$$|\chi^h|_1 \leq \frac{C}{h}|\chi^h|_h, \tag{2.26a}$$

$$\|\chi^h\|_{0,q} \leq Ch^{d(1/q-1/r)}\|\chi^h\|_{0,r}, \quad 1 \leq r \leq q \leq \infty, \tag{2.26b}$$

that hold for all $\chi^h \in S^h$, and an expression for the error due to numerical integration

$$|(\chi^h, \eta^h) - (\chi^h, \eta^h)^h| \leq Ch\|\chi^h\|_0|\eta^h|_1 \quad \forall \chi^h, \eta^h \in S^h, \tag{2.27}$$

[see the proof of [59, Lemma 15.1] and note the inverse inequality (2.26a)].

We recall several lemmata that are the discrete analogues of continuous theorems. To obtain error estimates in later sections we need a discrete Sobolev embedding result [19]:

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

$$|v|_{h,r} \leq C\|v\|_1 \quad \textit{for } r \in \begin{cases} [2,\infty] & \text{if } d = 1, \\ [2,\infty) & \text{if } d = 2, \\ [2,6] & \text{if } d = 3. \end{cases} \tag{2.28}$$

We also require a discrete Gagliardo–Nirenberg inequality [19] [cf. (1.6)]:

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

$$|v|_{h,r} \leq \frac{C}{h}|v|_h^{1-\mu}\|v\|_1^{\mu}, \tag{2.29}$$

where r is subject to the same restrictions as in Lemma 1.

To prove uniqueness of the semi discrete approximation we require the following lemma, which is similar to Lemma 3.4 in [19]:

Lemma 3 *Assume $\eta, \psi \in S^h$, $h \leq 1$, ε is a nonnegative real number, and the triangulation $\mathcal{T}^h$ is quasi-uniform. Then there are positive constants $C_h(\varepsilon) := C(\varepsilon)h^{2/(\mu-1)} > 0$, $\mu := d/4$, and C such that*

$$C\left(|\eta|, |\psi|^2\right)^h \leq \left(\frac{\mu}{\varepsilon} + C_h(\varepsilon)|\eta|_h^{\frac{1}{1-\mu}}\right)\|\psi\|_0^2 + \frac{\mu}{\varepsilon}|\psi|_1^2. \tag{2.30}$$

We give a 'modified' semi discrete approximation of (P):

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

$$(\mathbf{u}_t^h, \boldsymbol{\chi}^h)^h + a_\delta(\mathbf{u}^h, \boldsymbol{\chi}^h) = (\widehat{\mathbf{f}}(\mathbf{u}^h), \boldsymbol{\chi}^h)^h \quad \forall \boldsymbol{\chi}^h \in \mathbf{S}^h, \tag{2.31a}$$

where

$$\widehat{\mathbf{f}}(\mathbf{u}^h) \equiv \begin{pmatrix} \widehat{f}(u^h, v^h) \\ \widehat{g}(u^h, v^h) \end{pmatrix} := \begin{pmatrix} u^h(1-|u^h|) - v^h\,\widehat{h}(au^h) \\ b\,v^h\,\widehat{h}(au^h) - c\,v^h \end{pmatrix}, \tag{2.31b}$$

and $\mathbf{u}^h := (u^h, v^h)^T$, with the modified functional responses

$$\widehat{h}(\chi) = \widehat{h}_1(\chi) = \frac{\chi}{1+|\chi|}, \quad \text{with } a = 1/\alpha, b = \beta, c = \gamma, \tag{2.32a}$$

$$\widehat{h}(\chi) = \widehat{h}_2(\chi) = 1 - e^{-|\chi|}, \quad \text{with } a = \gamma, c = \beta, b = \alpha\beta. \tag{2.32b}$$

Lemma 4 *Let B be a convex compact subset of $\mathbb{R}^2$. Then*

$$|\widehat{\mathbf{f}}(\mathbf{u}_1) - \widehat{\mathbf{f}}(\mathbf{u}_2)| \le C\,(|\mathbf{u}_1| + |\mathbf{u}_2| + 1)\ |\mathbf{u}_1 - \mathbf{u}_2|, \quad \forall \mathbf{u}_1, \mathbf{u}_2 \in B. \tag{2.33}$$

Proof We write the modified reaction kinetics as

$$\widehat{\mathbf{f}}(\mathbf{u}) = \widehat{\mathbf{f}}_1(\mathbf{u}) + \widehat{\mathbf{f}}_2(\mathbf{u}) + \widehat{\mathbf{f}}_3(\mathbf{u}), \quad \mathbf{u} = (u, v)^T,$$

where

$$\widehat{\mathbf{f}}_1(\mathbf{u}) := \begin{pmatrix} 1 & 0 \\ 0 & -c \end{pmatrix}\mathbf{u}, \quad \widehat{\mathbf{f}}_2(\mathbf{u}) := \begin{pmatrix} -u|u| \\ 0 \end{pmatrix}, \quad \widehat{\mathbf{f}}_3(\mathbf{u}) := \begin{pmatrix} -v\,\widehat{h}(au) \\ b\,v\,\widehat{h}(au) \end{pmatrix}.$$

Noting that $\widehat{\mathbf{f}}_1(\mathbf{u})$ is linear and $|\widehat{\mathbf{f}}_2(\mathbf{u}_1) - \widehat{\mathbf{f}}_2(\mathbf{u}_2)| \le (|\mathbf{u}_1| + |\mathbf{u}_2|)|\mathbf{u}_1 - \mathbf{u}_2|$, a calculation yields that the spectral norm of the Jacobian matrix of $\widehat{\mathbf{f}}_3$ can be expressed as

$$\left\| \frac{\partial \widehat{\mathbf{f}}_3}{\partial \mathbf{z}} \right\|_2 = \sqrt{(1+b^2)\ \sup_s \left\{ a^2 z_2^2 \left(\frac{\partial \widehat{h}}{\partial \chi} \right)^2 + \left(\widehat{h}(\chi) \right)^2 \right\}}, \quad \chi := a z_1,$$

where $\mathbf{z} = (z_1, z_2)^T = (1-s)\mathbf{u}_1 + s\mathbf{u}_2$, $0 \le s \le 1$. This leads to the desired result as $\widehat{h}(\chi)$ and $\partial\widehat{h}/\partial\chi$ are strictly less then one. □

Before considering error estimates for the semi discrete approximation we need a stability lemma.

Lemma 5 *Let assumptions* (A^h) *hold,* $u_0, v_0 \in H^1(\Omega) \cap L^\infty(\Omega)$ *and* $h \le 1$, *then* (P^h) *possesses a unique solution* $\{u^h, v^h\}$ *such that the following stability bounds hold independent of* h:

$$u^h, v^h \in L^\infty(0, T; H^1(\Omega)) \cap L^\infty(0, T; L^{h,\infty}(\Omega)), \tag{2.34}$$

$$\frac{\partial u^h}{\partial t}, \frac{\partial v^h}{\partial t} \in L^2(\Omega_T). \tag{2.35}$$

Proof In (P^h) let $\mathbf{u}^h(\cdot,t) \equiv \mathbf{u}^h(t) = \sum_{i=0}^{J} \mathbf{U}_i(t)\varphi_i$ where $\mathbf{U}_i(t) \approx \mathbf{u}(\mathbf{x}_i,t)$ and take $\boldsymbol{\chi}^h = (\varphi_j, \varphi_j)^T$, $j = 0, \ldots, J$ to obtain $2J + 2$ ordinary differential equations. As $\widehat{\mathbf{f}}$ is a locally Lipschitz function, we conclude from standard ODE theory that the semi discrete approximation (P^h) has a unique solution on some finite time interval $(0, t_h)$, $t_h > 0$.

We derive below uniform (with respect to h) bounds of the semi discrete solutions via an a priori estimate, thus concluding $t_h = T$ independent of h. In addition, the first estimate leads to a generalised 'stability bound' for the semi discrete approximations.

Estimate I: Choose $\boldsymbol{\chi}^h = \left(\pi^h\{|u^h|^q u^h\}, \pi^h\{|v^h|^q v^h\}\right)^T$, $0 \le q < \infty$, in (2.31a) yielding

$$\begin{aligned} &\frac{1}{q+2}\frac{d}{dt}\left[|u^h|_{h,q+2}^{q+2} + |v^h|_{h,q+2}^{q+2}\right] \\ &\quad \le |u^h|_{h,q+2}^{q+2} - |u^h|_{h,q+3}^{q+3} + \left(|u^h|^{q+1}, |v^h|\right)^h + (b-c)|v^h|_{h,q+2}^{q+2}, \end{aligned} \tag{2.36}$$

where we noted

$$|\chi|^q \chi \frac{\partial \chi}{\partial t} = \frac{1}{q+2}\frac{\partial}{\partial t}|\chi|^{q+2} \quad (\chi = u^h,\ v^h), \quad |\widehat{h}(au^h)| < 1,$$

and (2.21). Applying (1.10) with $m = \frac{q+2}{q+1}$, $n = q + 2$, and $\varepsilon = 1$ to the third term on the RHS of (2.36) yields

$$\begin{aligned} &\frac{d}{dt}\left(|u^h|_{h,q+2}^{q+2} + |v^h|_{h,q+2}^{q+2}\right) + (q+2)|u^h|_{h,q+3}^{q+3} \\ &\quad \le (q+2)\, C_1(q)\left(|u^h|_{h,q+2}^{q+2} + |v^h|_{h,q+2}^{q+2}\right), \end{aligned}$$

where $C_1(q) := \max\left\{1 + \frac{q+1}{q+2}, \frac{1}{q+2} + b - c\right\}$. Applying the Grönwall lemma yields for a.e. $t \in (0, T)$

$$\begin{aligned} &|u^h(t)|_{h,q+2}^{q+2} + |v^h(t)|_{h,q+2}^{q+2} + (q+2)\int_0^t |u^h(s)|_{h,q+3}^{q+3}\, ds \\ &\quad \le \exp\{C_1(q)\,(q+2)t\}\left(|u^h(0)|_{h,q+2}^{q+2} + |v^h(0)|_{h,q+2}^{q+2}\right). \end{aligned}$$

We 'discard' the third term on the LHS, raise both sides to the power of $\frac{1}{q+2}$, and employ (1.11) to obtain

$$\begin{aligned} &|u^h(t)|_{h,q+2} + |v^h(t)|_{h,q+2} \\ &\quad \le 2^{\frac{q+1}{q+2}} \exp\{C_1(q)t\}\left(|u^h(0)|_{h,q+2} + |v^h(0)|_{h,q+2}\right). \end{aligned}$$

Applying the discrete injection result (2.20b), the projection property (2.22), and the assumption that $u_0, v_0 \in L^\infty(\Omega)$, we have

$$|u^h(t)|_{h,q+2} + |v^h(t)|_{h,q+2} \le C. \tag{2.37}$$

Note that for any $\chi^h \in S^h$ and $1 \le p < \infty$ we have

$$|\chi^h|_{h,p}^p = \sum_{j=0}^{J} \widehat{M}_{jj}|\chi^h(x_j)|^p \ge \max_{0\le j\le J} \left\{(\widehat{M}_{jj})^{1/p}|\chi^h(x_j)|\right\}^p,$$

so

$$\lim_{p\to\infty} |\chi^h|_{h,p} \ge |\chi^h|_{h,\infty}.$$

Hence from (2.37) we have

$$|u^h(t)|_{h,\infty} + |v^h(t)|_{h,\infty} \le C, \tag{2.38}$$

and consequently $u^h,\ v^h \in L^\infty(0, T; L^{h,\infty}(\Omega))$.

To show uniqueness let $\mathbf{u}^h$ and $\mathbf{v}^h$ be semi discrete solutions of (P^h). Set $\boldsymbol{\chi}^h = \mathbf{w}^h := \mathbf{u}^h - \mathbf{v}^h$ and subtract the semi discrete approximations to obtain after application of the Lipschitz condition (2.33), Lemma 3, and (1.16)

$$\frac{1}{2}\frac{d}{dt}|\mathbf{w}^h|_h^2 + c_\delta|\mathbf{w}^h|_1^2 \le C|\mathbf{w}^h|_h^2 + \left(C + C_h|\mathbf{u}^h|_h^\nu + C_h|\mathbf{v}^h|_h^\nu\right)\|\mathbf{w}^h\|_0^2 + \frac{\mu}{\varepsilon}|\mathbf{w}^h|_1^2,$$

where C_h is a positive constant depending on h, which we allow to change from expression to expression, and $\nu = 1/(1 - d/4)$. Taking $\varepsilon = \frac{2\mu}{c_\delta}$ gives

$$\frac{d}{dt}|\mathbf{w}^h|_h^2 + c_\delta|\mathbf{w}^h|_1^2 \le C|\mathbf{w}^h|_h^2 \left(1 + C_h|\mathbf{u}^h|_h^\nu + C_h|\mathbf{v}^h|_h^\nu\right).$$

Applying the Grönwall lemma yields for a.e. $t \in (0, T)$

$$\begin{aligned}
&|\mathbf{w}^h(t)|_h^2 \\
&\le |\mathbf{w}_0^h|_h^2 \exp\left\{Ct + C_h\left(\|\mathbf{u}^h\|^\nu_{L^\nu(0,T;L^{h,2}(\Omega))} + \|\mathbf{v}^h\|^\nu_{L^\nu(0,T;L^{h,2}(\Omega))}\right)\right\} \\
&\le |\mathbf{w}_0^h|_h^2 \exp\left\{Ct + C_h\left(\|\mathbf{u}^h\|^\nu_{L^\infty(0,T;L^{h,\infty}(\Omega))} + \|\mathbf{v}^h\|^\nu_{L^\infty(0,T;L^{h,\infty}(\Omega))}\right)\right\} \\
&\le C_h|\mathbf{w}_0^h|_h^2,
\end{aligned} \tag{2.39}$$

where $\mathbf{w}_0^h := \mathbf{w}^h(0) \equiv 0$, after noting (2.20b), $\nu \le 4$, and (2.38). Thus we conclude $\mathbf{u}^h \equiv \mathbf{v}^h$ as required.

Estimate II: This estimate is a discrete analogue of the continuous version. Substituting $\boldsymbol{\chi}^h = \mathbf{u}_t^h$ into (P^h), noting Young's inequality, $|\widehat{h}(\cdot)| < 1$, integrating over $(0, t)$, and applying (2.38) and (2.20b) leads to the remaining estimates. This completes the proof of Lemma 5. □

A semi discrete error bound

We estimate the error between the semi discrete solutions of (P^h) and the continuous solutions of (P).

Lemma 6 *Let the assumptions on the continuous solutions at the end of Sect.* 1 *and Lemma* 5 *hold. Then the semi discrete solution of* (P^h) *satisfies*:

$$\|\mathbf{u}-\mathbf{u}^h\|_{L^\infty(0,T;L^2(\Omega))}+\|\mathbf{u}-\mathbf{u}^h\|_{L^2(0,T;H^1(\Omega))}\leq Ch. \tag{2.40}$$

Proof Set $\mathbf{e}:=\mathbf{u}-\mathbf{u}^h$, $\mathbf{e}^A:=\mathbf{u}-\pi^h\mathbf{u}$, and $\mathbf{e}^h=\pi^h\mathbf{u}-\mathbf{u}^h$. Choosing $\boldsymbol{\eta}=\mathbf{e}^h$ in (P), $\boldsymbol{\chi}^h=\mathbf{e}^h$ in (P^h), and subtracting leads to

$$(\mathbf{u}_t,\mathbf{e}^h)-(\mathbf{u}^h_t,\mathbf{e}^h)^h+a_\delta(\mathbf{e},\mathbf{e}^h)=(\mathbf{f}(\mathbf{u}),\mathbf{e}^h)-(\widehat{\mathbf{f}}(\mathbf{u}^h),\mathbf{e}^h)^h. \tag{2.41}$$

Adding and subtracting each of the terms $(\mathbf{u}^h_t,\mathbf{e}^h)$ and $(\widehat{\mathbf{f}}(\mathbf{u}),\mathbf{e}^h)$ to (2.41), noting (1.16), and rearranging yields

$$\frac{1}{2}\frac{d}{dt}\|\mathbf{e}\|_0^2+c_\delta|\mathbf{e}|_1^2\leq\left\{(\mathbf{u}^h_t,\mathbf{e}^h)^h-(\mathbf{u}^h_t,\mathbf{e}^h)\right\}+\left(\frac{\partial\mathbf{e}}{\partial t},\mathbf{e}^A\right)+a_\delta(\mathbf{e},\mathbf{e}^A)$$
$$+(\mathbf{f}(\mathbf{u})-\widehat{\mathbf{f}}(\mathbf{u}^h),\mathbf{e}^h)+\left\{(\widehat{\mathbf{f}}(\mathbf{u}^h),\mathbf{e}^h)-(\widehat{\mathbf{f}}(\mathbf{u}^h),\mathbf{e}^h)^h\right\}=:\sum_{i=1}^{5}T_i. \tag{2.42}$$

With the aid of the (1.10), (2.27), (2.25a), (2.33), (2.38), and the Cauchy–Schwarz inequality we easily bound the first four terms:

$$T_1\leq Ch^2\|\mathbf{u}^h_t\|_0^2+\frac{1}{\varepsilon_1}|\mathbf{e}|_1^2+Ch^2\|\mathbf{u}\|_2^2, \tag{2.43}$$

$$T_2\leq Ch^2\|\mathbf{u}\|_2\left\|\frac{\partial\mathbf{e}}{\partial t}\right\|_0, \tag{2.44}$$

$$T_3\leq Ch^2\|\mathbf{u}\|_2^2+\frac{1}{2\varepsilon_2}|\mathbf{e}|_1^2, \tag{2.45}$$

$$T_4\leq C\|\mathbf{e}\|_0^2+Ch^4\|\mathbf{u}\|_2^2. \tag{2.46}$$

Estimating the final term is more technical. Recalling (2.25b) we have

$$T_5\leq\int_\Omega\left|(I-\pi^h)\left(\widehat{\mathbf{f}}(\mathbf{u}^h)\cdot\mathbf{e}^h\right)\right|\,dx$$
$$\leq Ch^2\sum_{i,j=1}^{d}\int_\Omega\left|\frac{\partial^2\left(\widehat{\mathbf{f}}(\mathbf{u}^h)\cdot\mathbf{e}^h\right)}{\partial x_i\partial x_j}\right|\,dx=:T_{5,1}. \tag{2.47}$$

To avoid taking second derivatives of piecewise linear functions we initially estimate the RHS of (2.47) on a single reference triangle τ. First note

$$\left|\frac{\partial^2\left(\widehat{\mathbf{f}}(\mathbf{u}^h)\cdot\mathbf{e}^h\right)}{\partial x_i\partial x_j}\right| = \left|\frac{\partial\widehat{\mathbf{f}}(\mathbf{u}^h)}{\partial x_j}\cdot\frac{\partial\mathbf{e}^h}{\partial x_i}+\mathbf{e}^h\cdot\frac{\partial^2\widehat{\mathbf{f}}(\mathbf{u}^h)}{\partial x_i\partial x_j}+\frac{\partial\widehat{\mathbf{f}}(\mathbf{u}^h)}{\partial x_i}\cdot\frac{\partial\mathbf{e}^h}{\partial x_j}\right|$$
$$\leq \left|\frac{\partial\mathbf{e}^h}{\partial x_i}\right|\left\{\left|\frac{\partial\widehat{f}}{\partial x_j}\right|+\left|\frac{\partial\widehat{g}}{\partial x_j}\right|\right\}+|\mathbf{e}^h|\left\{\left|\frac{\partial^2\widehat{f}}{\partial x_i\partial x_j}\right|+\left|\frac{\partial^2\widehat{g}}{\partial x_i\partial x_j}\right|\right\}$$
$$+\left|\frac{\partial\mathbf{e}^h}{\partial x_j}\right|\left\{\left|\frac{\partial\widehat{f}}{\partial x_i}\right|+\left|\frac{\partial\widehat{g}}{\partial x_i}\right|\right\}. \tag{2.48}$$

It follows from (2.38) and $\widehat{h}(au^h)\leq 1$ that

$$\left|\frac{\partial\widehat{f}}{\partial x_i}\right|,\ \left|\frac{\partial\widehat{g}}{\partial x_i}\right|\leq C\left(\left|\frac{\partial u^h}{\partial x_i}\right|+\left|\frac{\partial v^h}{\partial x_i}\right|\right)+C|H(u^h)|\left|\frac{\partial u^h}{\partial x_i}\right|, \tag{2.49}$$

$$\left|\frac{\partial^2\widehat{f}}{\partial x_i\partial x_j}\right|,\ \left|\frac{\partial^2\widehat{g}}{\partial x_i\partial x_j}\right|$$
$$\leq C|H(u^h)|\left\{\left|\frac{\partial u^h}{\partial x_i}\right|\left|\frac{\partial u^h}{\partial x_j}\right|+\left|\frac{\partial u^h}{\partial x_i}\right|\left|\frac{\partial v^h}{\partial x_j}\right|+\left|\frac{\partial u^h}{\partial x_j}\right|\left|\frac{\partial v^h}{\partial x_i}\right|\right\}$$
$$+C\left|\frac{\partial H(u^h)}{\partial x_j}\right|\left|\frac{\partial u^h}{\partial x_i}\right|+C\left|\frac{\partial u^h}{\partial x_i}\right|\left|\frac{\partial v^h}{\partial x_j}\right|+C\left|\frac{\partial u^h}{\partial x_j}\right|\left|\frac{\partial v^h}{\partial x_i}\right|, \tag{2.50}$$

where $H(u^h)$ is a Heaviside type distribution, symbolically represented by

$$H(u^h)=\begin{cases}+1 & \text{if } u^h>0 \text{ on } \tau,\\ -1 & \text{if } u^h<0 \text{ on } \tau.\end{cases}$$

Thus combining (2.48)–(2.50) and applying Hölder's inequality leads to

$$Ch_\tau^2\sum_{i,j=1}^{d}\int_\tau\left|\frac{\partial^2\left(\widehat{\mathbf{f}}(\mathbf{u}^h)\cdot\mathbf{e}^h\right)}{\partial x_i\partial x_j}\right|dx$$
$$\leq Ch_\tau^2\sum_{i,j=1}^{d}\left\{\|\mathbf{e}^h\|_{1,\tau}\left(\|u^h\|_{1,\tau}+\|v^h\|_{1,\tau}\right)\right.$$
$$+\|\mathbf{e}^h\|_{0,\infty,\tau}\|u^h\|_{1,\tau}^2+\|\mathbf{e}^h\|_{0,\infty,\tau}\|u^h\|_{1,\tau}\|v^h\|_{1,\tau}$$
$$\left.+\|\mathbf{e}^h\|_{0,\infty,\tau}\left\|\left|\frac{\partial u^h}{\partial x_i}\right|\left|\frac{\partial u^h}{\partial x_j}\right|\right\|_{2,\tau}\|\delta(u^h)\|_{-2,\tau}\right\}, \tag{2.51}$$

where $\delta(u^h)$ is a Dirac delta type distribution, symbolically represented by

$$\delta(u^h) = \begin{cases} 0 & \text{if } u^h \neq 0 \text{ on } \tau, \\ \infty & \text{if } u^h = 0 \text{ on } \tau. \end{cases}$$

Recalling (1.5) and noting that the Dirac delta distribution acts on point values, we need $u^h \in H^{\frac{d}{2}+\varepsilon}(\tau)$ to have $\delta(u^h) \in H^{-\left(\frac{d}{2}+\varepsilon\right)}(\tau)$. Thus it is sufficient to have $u^h \in H^2(\tau)$ and take $\delta(u^h) \in H^{-2}(\tau)$ as $d \leq 3$. To estimate the RHS of (2.51) we use $\|\mathbf{e}^h\|_{0,\infty,\tau} \leq C h_\tau^{-1/2} \|\mathbf{e}^h\|_{1,\tau}$, which follows from the inverse inequality (2.26b) together with the Sobolev Embedding Theorem (1.4) with $q = 4$ when $d = 2$ and $q = 6$ when $d = 3$. Furthermore, as $\partial u^h/\partial x_i$, $\partial v^h/\partial x_j$ are constant on τ, we have with the aid of the Sobolev Embedding Theorem

$$\begin{aligned} \left\| \left|\frac{\partial u^h}{\partial x_i}\right| \left|\frac{\partial u^h}{\partial x_j}\right| \right\|_{2,\tau} \equiv \left\| \left|\frac{\partial u^h}{\partial x_i}\right| \left|\frac{\partial u^h}{\partial x_j}\right| \right\|_{0,\tau} &\leq \left\| \frac{\partial u^h}{\partial x_i} \right\|_{0,4,\tau} \left\| \frac{\partial u^h}{\partial x_j} \right\|_{0,4,\tau} \\ &\leq C \|u^h\|_{1,\tau}^2. \end{aligned}$$

Thus using (2.25a), (2.34), (1.10), and summing the contributions from all simplices, yields

$$T_{5,1} \leq Ch^2 + C\|\mathbf{e}\|_0^2 + \frac{1}{\varepsilon_3}|\mathbf{e}|_1^2 + Ch^2\|\mathbf{u}\|_2^2. \tag{2.52}$$

Combining (2.42)–(2.47), (2.52), and taking $\varepsilon_1 = \varepsilon_2 = \varepsilon_3 = \frac{5}{c_\delta}$ leads to

$$\frac{d}{dt}\|\mathbf{e}\|_0^2 + c_\delta|\mathbf{e}|_1^2 \leq C\|\mathbf{e}\|_0^2 + Ch^2\left(1 + \|\mathbf{u}\|_2^2 + \|\mathbf{u}\|_2 \left\|\frac{\partial \mathbf{e}}{\partial t}\right\|_0 + \|\mathbf{u}_t^h\|_0^2\right). \tag{2.53}$$

Applying the Grönwall lemma and the Cauchy–Schwarz inequality yields for a.e. $t \in (0, T)$

$$\begin{aligned} &\|\mathbf{e}(t)\|_0^2 + c_\delta \int_0^t |\mathbf{e}(s)|_1^2\, ds \\ &\quad \leq C\|\mathbf{e}(0)\|_0^2 + Ch^2\Bigg(t + \|\mathbf{u}_t^h\|_{L^2(\Omega_t)}^2 + \|\mathbf{u}\|_{L^2(0,t;H^2(\Omega))}^2 \\ &\qquad + \|\mathbf{u}\|_{L^2(0,t;H^2(\Omega))}\left\|\frac{\partial \mathbf{e}}{\partial t}\right\|_{L^2(\Omega_t)}\Bigg) \leq Ch^2, \end{aligned}$$

where we noted (2.23), (2.35), the assumptions on the continuous solutions at the end of Sect. 1, and the $\mathbf{H}^1$ bound on the initial data. The result follows. □

3 Fully discrete approximations

In what follows N is a positive integer, $\Delta t := T/N$ is the time step, and $t_n := n\,\Delta t$. We study the following fully discrete, semi implicit in time, finite element approximation of problem (P):

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

$$\left(\frac{\mathbf{U}^n - \mathbf{U}^{n-1}}{\Delta t}, \boldsymbol{\chi}^h\right)^h + a_\delta(\mathbf{U}^n, \boldsymbol{\chi}^h) = (\widetilde{\mathbf{f}}(\mathbf{U}^n, \mathbf{U}^{n-1}), \boldsymbol{\chi}^h)^h \quad \forall \boldsymbol{\chi}^h \in \mathbf{S}^h, \tag{3.54a}$$

where

$$\widetilde{\mathbf{f}}(\mathbf{U}^n, \mathbf{U}^{n-1}) := \begin{pmatrix} U^n(1 - |U^{n-1}|) - V^n\,\widehat{h}(aU^{n-1}) \\ b\,V^n\,\widehat{h}(aU^{n-1}) - c\,V^n \end{pmatrix}, \tag{3.54b}$$

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

We require the following discrete Grönwall lemma [18, Lemma 5.1.1].

Lemma 7 *Assume $w_n, \alpha_n, p_n \geq 0$, $0 \leq \beta < 1$, satisfy*

$$w_n + p_n \leq \alpha_n + \beta \sum_{k=0}^{n-1} w_{k+1}, \quad \forall n \geq 0, \tag{3.55}$$

where $\{\alpha_n\}$ is nondecreasing $\left(\text{with the convention that } \sum_{k=0}^{-1}(\cdot) = 0\right)$. Then

$$w_n + \frac{p_n}{1-\beta} \leq \left(\frac{\alpha_n - \beta w_0}{1-\beta}\right) \exp\left(\frac{n\beta}{1-\beta}\right). \tag{3.56}$$

The following theorem is the main theoretical result of this paper.

Theorem 1 *Let the assumptions of Lemma 6 hold, and assume the time step satisfies $\Delta t < \min\left\{\frac{1}{7}, \frac{1}{1+4(b-c)}\right\}$, $(b > c)$. Then there exists a unique solution of $\left(\mathrm{P}_1^{h,\Delta t}\right)$ such that*

$$\Delta t \max_{1\leq n\leq N} \|\mathbf{U}^n\|_1 + \Delta t \sum_{n=1}^{N} |\mathbf{U}^n - \mathbf{U}^{n-1}|_1^2 + \sum_{n=1}^{N} |\mathbf{U}^n - \mathbf{U}^{n-1}|_h^2 \leq C\Delta t. \tag{3.57}$$

Furthermore, we have

$$\|\mathbf{u} - \mathbf{U}^+\|_{L^\infty(0,T;L^2(\Omega))} + \|\mathbf{u} - \mathbf{U}^+\|_{L^2(0,T;H^1(\Omega))} \leq C(\Delta t^{1/2} + h), \tag{3.58}$$

where

$$\mathbf{U}^{+}(t) := \mathbf{U}^{n}, \quad t \in (t_{n-1}, t_n],\ n \geq 1. \tag{3.59}$$

Proof The existence and uniqueness of solutions to the fully discrete finite element scheme ($\mathrm{P}_1^{h,\Delta t}$) follows from Lemma 8 (see Sect. 4). To deduce (3.57) we require two additional stability estimates.

Estimate III: The estimate is a fully discrete analogue of Estimate I with $q = 2$. Choose $\chi^h = (\pi^h\{|U^n|^2 U^n\}, \pi^h\{|V^n|^2 V^n\})^T$ in (3.54a). Then noting (1.9), (2.21), and $\widehat{h}(\cdot) < 1$ yields

$$\begin{aligned}\frac{1}{4\Delta t}&\left[\left(|U^n|_{h,4}^4 + |V^n|_{h,4}^4\right) - \left(|U^{n-1}|_{h,4}^4 + |V^{n-1}|_{h,4}^4\right)\right]\\ &\leq |U^n|_{h,4}^4 - (|U^n|^4, |U^{n-1}|)^h + (|U^n|^3, |V^n|)^h + (b-c)|V^n|_{h,4}^4.\end{aligned} \tag{3.60}$$

Applying the Young's inequality (1.10) with $m = \frac{4}{3}$, $n = 4$, and $\varepsilon = 1$ yields

$$\begin{aligned}&\left[\left(|U^n|_{h,4}^4 + |V^n|_{h,4}^4\right) - \left(|U^{n-1}|_{h,4}^4 + |V^{n-1}|_{h,4}^4\right)\right] + 4\Delta t(|U^n|^4, |U^{n-1}|)^h\\ &\quad\leq 4C_2\Delta t\left(|U^n|_{h,4}^4 + |V^n|_{h,4}^4\right),\end{aligned} \tag{3.61}$$

where $C_2 := \max\{\frac{7}{4}, \frac{1}{4} + b - c\}$. Changing notation from n to i we sum over all $i = 1, \ldots, n$ and apply the discrete Grönwall lemma yielding

$$\begin{aligned}|U^n|_{h,4}^4 + |V^n|_{h,4}^4 &+ \left(\frac{4\Delta t}{1 - 4C_2\,\Delta t}\right)\sum_{i=1}^{n}(|U^i|^4, |U^{i-1}|)^h\\ &\leq \left(|U^0|_{h,4}^4 + |V^0|_{h,4}^4\right)\exp\left(\frac{4C_2\,t_n}{1 - 4C_2\,\Delta t}\right) \quad (t_n \equiv n\Delta t),\end{aligned}$$

where we note that $\Delta t < 1/(4C_2)$ by assumption. After applying the discrete Sobolev embedding result $|\chi|_{h,4} \leq C\|\chi\|_1$ ($\chi = U^0, V^0$) [see (2.28)] and recalling that the initial data is in $H^1(\Omega)$ we deduce the following uniform bounds:

$$\max_{1\leq n\leq N} |U^n|_{h,4}, \ \max_{1\leq n\leq N} |V^n|_{h,4} \leq C. \tag{3.62}$$

From (2.20b) it follows that $|\cdot|_h \leq C|\cdot|_{h,4}$, and so we also have

$$\max_{1\leq n\leq N} |U^n|_{h}, \ \max_{1\leq n\leq N} |V^n|_{h} \leq C. \tag{3.63}$$

Estimate IV: The estimate is a fully discrete analogue of Estimate II. Choose $\boldsymbol{\chi}^h = (\mathbf{U}^n - \mathbf{U}^{n-1})/\Delta t$ in (3.54a). Then noting the elementary identity

$$2b(b-a) \equiv |b-a|^2 + b^2 - a^2 \quad \forall a, b,$$

Young's inequality, and (2.20a) leads to

$$\Delta t \left| \frac{\mathbf{U}^n - \mathbf{U}^{n-1}}{\Delta t} \right|_h^2 + |\mathbf{U}^n - \mathbf{U}^{n-1}|_{a_\delta}^2 + |\mathbf{U}^n|_{a_\delta}^2 - |\mathbf{U}^{n-1}|_{a_\delta}^2$$
$$\leq C\Delta t |\mathbf{U}^n|_h^2 + C\Delta t |\mathbf{U}^n|_{h,4}^2 |\mathbf{U}^{n-1}|_{h,4}^2. \quad (3.64)$$

Applying bounds (3.62) and (3.63) we see that the RHS of (3.64) is bounded by $C\Delta t$. After a change of notation from n to i, summing over all $i = 1, \ldots, n$, noting (1.16), the projection property (2.24), and the $\mathbf{H}^1(\Omega)$ bound on the initial data yields

$$\Delta t \sum_{i=1}^{n} \left| \frac{\mathbf{U}^i - \mathbf{U}^{i-1}}{\Delta t} \right|_h^2 + c_\delta \sum_{i=1}^{n} |\mathbf{U}^i - \mathbf{U}^{i-1}|_1^2 + c_\delta |\mathbf{U}^n|_1^2$$
$$\leq C_\delta |\mathbf{U}^0|_1^2 + C t_n \leq C.$$

This leads to (3.57) after noting (3.63).

The prove of the fully discrete error bound (3.58) is similar to that given in [19], and so only minimal details are provided here. Define

$$\mathbf{U}^-(t) := \mathbf{U}^{n-1}, \quad t \in (t_{n-1}, t_n],\ n \geq 1, \quad (3.65)$$
$$\mathbf{U}(t) := \left(\frac{t - t_{n-1}}{\Delta t} \right) \mathbf{U}^n + \left(\frac{t_n - t}{\Delta t} \right) \mathbf{U}^{n-1}, \quad t \in [t_{n-1}, t_n],\ n \geq 1,$$

and note

$$\frac{\partial \mathbf{U}}{\partial t} = \frac{\mathbf{U}^+ - \mathbf{U}^-}{\Delta t} = \frac{\mathbf{U} - \mathbf{U}^-}{t - t_{n-1}} = \frac{\mathbf{U}^+ - \mathbf{U}}{t_n - t}, \quad t \in (t_{n-1}, t_n],\ n \geq 1. \quad (3.66)$$

Thus we can restate the fully discrete scheme as:

Find $\mathbf{U} \in \{H^1(0, T; S^h)\}^2$ such that $\mathbf{U}(\cdot, 0) := Q^h \mathbf{u}_0(\cdot)$ and for a.e. $t \in (0, T)$

$$\left(\frac{\partial \mathbf{U}}{\partial t}, \boldsymbol{\chi}^h \right)^h + a_\delta(\mathbf{U}^+, \boldsymbol{\chi}^h) = (\tilde{\mathbf{f}}(\mathbf{U}^+, \mathbf{U}^-), \boldsymbol{\chi}^h)^h \quad \forall \boldsymbol{\chi}^h \in \mathbf{S}^h. \quad (3.67)$$

Define $\mathbf{E}^+ := \mathbf{u}^h - \mathbf{U}^+ \in \mathbf{S}^h$, $\mathbf{E} := \mathbf{u}^h - \mathbf{U} \in \mathbf{S}^h$, and $\mathbf{E}^- := \mathbf{u}^h - \mathbf{U}^- \in \mathbf{S}^h$. Subtracting (2.31a) from (3.67) with $\boldsymbol{\chi}^h = \mathbf{E}^+$ yields

$$\left(\frac{\partial \mathbf{E}}{\partial t}, \mathbf{E}^+ \right)^h + c_\delta |\mathbf{E}^+|_1^2 \leq (\widehat{\mathbf{f}}(\mathbf{u}^h) - \tilde{\mathbf{f}}(\mathbf{U}^+, \mathbf{U}^-), \mathbf{E}^+)^h,$$

[recall (2.31b)], which we rewrite as

$$\frac{1}{2}\frac{d}{dt}|\mathbf{E}|_h^2 + c_\delta|\mathbf{E}^+|_1^2 \leq \left(\frac{\partial \mathbf{E}}{\partial t}, \mathbf{U}^+ - \mathbf{U}\right)^h + (\widehat{\mathbf{f}}(\mathbf{u}^h) - \tilde{\mathbf{f}}(\mathbf{U}^+, \mathbf{U}^-), \mathbf{E}^+)^h$$
$$\equiv I_1 + I_2. \tag{3.68}$$

Noting (2.20a), (2.33), a three-term version of (2.20a), (2.34), (2.28), and the Young's inequality (1.10) yields

$$I_1 \leq \left|\frac{\partial \mathbf{u}^h}{\partial t}\right|_h |\mathbf{U}^+ - \mathbf{U}^-|_h + \frac{1}{\Delta t}|\mathbf{U}^+ - \mathbf{U}^-|_h^2, \tag{3.69}$$

$$I_2 \leq C\left(|\mathbf{E}|_h^2 + |\mathbf{U}^+ - \mathbf{U}^-|_h^2\right) + \frac{1}{2\varepsilon}|\mathbf{E}^+|_1^2. \tag{3.70}$$

After taking $\varepsilon = \frac{1}{c_\delta}$, noting the Grönwall lemma, (3.57), (2.35), and Lemma 6, the remainder of the proof is as in [19]. □

Remark 1 Consider taking $\boldsymbol{\chi}^h = \mathbf{U}^n$ in (3.54a). Proceeding in a similar fashion to Estimate III leads to a stability estimate with the condition that

$$\Delta t < \min\left\{\tfrac{1}{3}, \tfrac{1}{1+2(b-c)}\right\} \leq \tfrac{1}{3}, \quad (b > c).$$

This is an improvement on the time step restriction needed in Estimate III.

Remark 2 We were unable to mimic a generalised version of Estimate I in the fully discrete case (Estimate III is the analogue of Estimate I with $q = 2$). The reason for this is that as q increases, the condition on Δt becomes increasingly more restrictive, until at the limit ($q = \infty$) we need $\Delta t \leq 0$ for stability, which is absurd.

Remark 3 We proved that the following alternative fully discrete finite element method satisfies the same stability and convergence results as $(\mathbf{P}_1^{h,\Delta t})$ (details omitted for the sake of brevity):

$(\mathbf{P}_2^{h,\Delta t})$ For $n = 1, \ldots, N$ find $\mathbf{U}^n \in \mathbf{S}^h$ such that $\mathbf{U}^0 := Q^h\mathbf{u}_0$ and

$$\left(\frac{\mathbf{U}^n - \mathbf{U}^{n-1}}{\Delta t}, \boldsymbol{\chi}^h\right)^h + a_\delta(\mathbf{U}^n, \boldsymbol{\chi}^h) = (\widehat{\mathbf{f}}(\mathbf{U}^{n-1}), \boldsymbol{\chi}^h)^h \quad \forall \boldsymbol{\chi}^h \in \mathbf{S}^h,$$

where

$$\widehat{\mathbf{f}}(\mathbf{U}^{n-1}) := \begin{pmatrix} U^{n-1}(1 - |U^{n-1}|) - V^{n-1}\,\widehat{h}(aU^{n-1}) \\ b\,V^{n-1}\,\widehat{h}(aU^{n-1}) - c\,V^{n-1} \end{pmatrix},$$

$\mathbf{U}^n = (U^n, V^n)^T$, and $\widehat{h}(\cdot)$ is as in (2.32a) or (2.32b). Note that the approximation of the kinetics in $(\mathbf{P}_2^{h,\Delta t})$ is entirely at the previous time level. It is advantageous to have a second method that satisfies the same theoretical results as it provides an additional test of convergence in the numerical computations (see next section).

4 Numerical results

Before presenting numerical results in one and two space dimensions, we discuss some properties of the resulting linear system, and numerically verify the rates of convergence in one space dimension. The linear systems resulting from the solution of the one dimensional problems were solved using direct methods, while in the two dimensional case we solved the linear systems using the GMRES algorithm (without preconditioning or 'restarting'). We used a uniform mesh, with fixed time steps, and in the two dimensional case a 'right-angled' triangulation of the square with the natural numbering of the nodes. Our criterion for deciding when numerical solutions converged, was to compare solutions from scheme $\left(\mathbf{P}_1^{h,\Delta t}\right)$ with those from scheme $\left(\mathbf{P}_2^{h,\Delta t}\right)$ (see Remark 3) and reduce the time and space steps until the difference between solutions was virtually indistinguishable.

Choosing $U^n = \sum_{j=0}^{J} U_j^n \varphi_j$, $V^n = \sum_{j=0}^{J} V_j^n \varphi_j$, $\chi^h = \varphi_i$, $i = 0, \dots J$, in $(\mathrm{P}_1^{h,\Delta t})$, where $U_j^n \approx u\big(\mathbf{x}_j, n\Delta t\big)$ and $V_j^n \approx v(\mathbf{x}_j, n\Delta t)$, leads to the following block matrix form of $(2J+2)$ linear equations for $n = 1, \dots, N$:

$$\begin{pmatrix} A_{n-1} & B_{n-1} \\ 0 & C_{n-1} \end{pmatrix} \begin{pmatrix} \mathcal{U}^n \\ \mathcal{V}^n \end{pmatrix} = \begin{pmatrix} \mathcal{U}^{n-1} \\ \mathcal{V}^{n-1} \end{pmatrix}, \quad \mathcal{U}^0 := (\widehat{M})^{-1}\mathcal{U}_0, \quad \mathcal{V}^0 := (\widehat{M})^{-1}\mathcal{V}_0, \tag{4.72}$$

where

$$\begin{aligned}
A_{n-1} &:= (1-\Delta t)I + \Delta t \ \mathrm{diag}\{|U_0^{n-1}|, \dots, |U_J^{n-1}|\} + \Delta t\, \widehat{M}^{-1}K, \\
B_{n-1} &:= \Delta t \ \mathrm{diag}\{\widehat{h}(aU_0^{n-1}), \dots, \widehat{h}(aU_J^{n-1})\}, \\
C_{n-1} &:= (1+\Delta t\, c)I - \Delta t\, b\, \mathrm{diag}\{\widehat{h}(aU_0^{n-1}), \dots, \widehat{h}(aU_J^{n-1})\} + \delta \Delta t\, \widehat{M}^{-1}K, \\
\mathcal{U}^n &:= (U_0^n, \dots, U_J^n)^T, \quad \mathcal{V}^n := (V_0^n, \dots, V_J^n)^T, \\
\{\mathcal{U}_0\}_i &:= (u_0, \varphi_i), \quad \{\mathcal{V}_0\}_i := (v_0, \varphi_i).
\end{aligned}$$

At each time step we solve the above system in two stages. First we solve $C_{n-1}\mathcal{V}^n = \mathcal{V}^{n-1}$ for $\mathcal{V}^n$, and then solve $A_{n-1}\mathcal{U}^n = \mathcal{U}^{n-1} - B_{n-1}\mathcal{V}^n$ for $\mathcal{U}^n$.

Lemma 8 *With the assumption on Δt in Theorem 1, the coefficient matrix of the linear system (4.72) is strictly (row) diagonally dominant.*

Proof From the weak acuteness property of the partitioning of Ω it follows that

$$\sum_{\substack{j=0 \\ j\neq i}}^{J} |L_{ij}| = L_{ii}, \quad \text{where } L_{ij} := (\widehat{M}_{ii})^{-1}K_{ij}. \tag{4.73}$$

Consider rows $0 \le i \le J$. By assumption $\Delta t < 1/2$ and recalling $\widehat{h}(\cdot) < 1$ we have

$$1 - \Delta t + \Delta t\,|U_i^{n-1}| + \Delta t\, L_{ii} > \Delta t \sum_{\substack{j=0\\ j\neq i}}^{J} |L_{ij}| + \Delta t\, \widehat{h}(aU_i^{n-1}).$$

Similarly, as by assumption $\Delta t < 1/(b-c)$, it holds for rows $J+1 \le i \le 2J+2$ that

$$1 + \Delta t\, c - \Delta t\, b\, \widehat{h}(aU_i^{n-1}) + \delta \Delta t\, L_{ii} > \delta \Delta t \sum_{\substack{j=0\\ j\neq i}}^{J} |L_{ij}|,$$

and the result follows. □

Remark 4 With the condition on Δt in Remark 1, the above Lemma still holds.

Remark 5 If the initial data $\{u_0, v_0\}$ is in $H^2(\Omega)$ (and hence in $C(\bar{\Omega})$ for $d \le 3$) we can choose our initial approximations $U^0 = \pi^h u_0$, $V^0 = \pi^h v_0$. In the fully discrete estimates we can then bound the initial data with the aid of the usual interpolation error estimate (2.25a), for example:

$$\|\pi^h u_0\|_1 \le \|\pi^h u_0 - u_0\|_1 + \|u_0\|_1 \le Ch|u_0|_2 + C \le C.$$

We present numerical evidence in one space dimension for the prey u using Kinetics (i) that verifies the error bound (3.58). As no exact solution of (P) is known, we compared computed solutions on a fine mesh and a small time step, with the corresponding approximations on a sequence of coarse meshes and larger time steps. Similar results were obtained for Kinetics (ii) (results omitted).

Let u^n be the approximate solution on the fine mesh with space-step h_{fine} and N_{fine} time steps Δt_{fine}, and U^n be the approximation on a coarse grid with space-step h and N time steps Δt. Define

$$\begin{aligned} u^+(t) &:= u^n, \qquad t \in (t_{n-1}, t_n], \quad t_n := n\Delta t_{fine}, \quad 1 \le n \le N_{fine},\\ U^+(t) &:= U^n, \qquad t \in (t_{n-1}, t_n], \quad t_n := n\Delta t, \quad 1 \le n \le N, \end{aligned}$$

then it is easy to see with the aid of the triangle inequality and the fully discrete error bound (3.58) that

$$\|u^+ - U^+\|_{L^\infty(0,T;L^2(\Omega))} + \|u^+ - U^+\|_{L^2(0,T;H^1(\Omega))} \le C(\Delta t^{1/2} + h). \tag{4.74}$$

This error bound can be evaluated exactly, since for all $v^h \in S^h$

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

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

$$\xi_0(h, \Delta t) = \|u^+ - U^+\|^2_{L^2(0,T;H^1(\Omega))} = \Delta t \sum_{n=1}^{N} \left(\|u^n - U^n\|_0^2 + |u^n - U^n|_1^2 \right), \quad (4.75)$$

$$\xi_\infty(h, \Delta t) = \|u^+ - U^+\|^2_{L^\infty(0,T;L^2(\Omega))} \equiv \max_{1 \le n \le N} \|u^n - U^n\|_0^2. \quad (4.76)$$

To verify (4.74) we used a uniform partition of $\Omega = (0, L), 0 \le t \le T$, with $x_j = jh$, $j = 0, \ldots, J$, where $h := L/J$. We fixed $h_{fine} = 1/1024$, $\Delta t_{fine} = 1/57344$, $L = 50$, $T = 10/7$, $\alpha = 0.3$, $\beta = 2.0$, $\gamma = 0.8$, and chose the initial data

$$u(x, 0) = u^* + u^* \cos(\pi x/16),$$
$$v(x, 0) = v^* + v^* \sin(\pi x/16),$$

where $u^* = 0.2$, $v^* = 0.4$ [recall (1.3a)]. We computed the ratios

$$R_i^h := \frac{\xi_i(h, \Delta t) - \xi_i(h/2, \Delta t)}{\xi_i(h/2, \Delta t) - \xi_i(h/4, \Delta t)}, \quad R_i^{\Delta t} := \frac{\xi_i(h, \Delta t) - \xi_i(h, \Delta t/2)}{\xi_i(h, \Delta t/2) - \xi_i(h, \Delta t/4)}, \quad (4.77)$$

($i = 0, \infty$), to obtain the results in Tables 1 and 2.

Writing the quantities $\xi_0(h, \Delta t)$ and $\xi_\infty(h, \Delta t)$ in the form

$$ah^p + A(\Delta t)^q, \quad p, q, a, A \in \mathbb{R},$$

and simplifying the ratios in (4.77) yields $R_i^h = 2^p$ and $R_i^{\Delta t} = 2^q$ ($i = 0, \infty$). The tabulated results indicate that the rate of convergence is $\mathcal{O}(h + \Delta t)$, which is consistent with the error bound (3.58).

Table 1 Verification of (4.74): $\Delta t = \frac{1}{7(2^{13})}$, $h = \frac{1}{2^j}$, $j = 0, 1, 2, 3, 4$

h	$\xi_0(h, 1/57344)$	$\xi_\infty(h, 1/57344)$	R_0^h	R_∞^h
1	2.506e−05	1.724e−05	14.4	16.3
1/2	1.763e−06	1.060e−06	12.5	16.1
1/4	1.424e−07	6.605e−08	11.1	15.7
1/8	1.303e−08	4.475e−09	–	–
1/16	1.329e−09	5.548e−10	–	–

Table 2 Verification of (4.74): $h = \frac{1}{2^{10}}$, $\Delta t = \frac{1}{7(2^j)}$, $j = 0, 1, 2, 3, 4$

Δt	$\xi_0(1/1024, \Delta t)$	$\xi_\infty(1/1024, \Delta t)$	$R_0^{\Delta t}$	$R_\infty^{\Delta t}$
1/7	8.301e−03	1.154e−02	4.84	4.48
1/14	1.757e−03	2.618e−03	4.40	4.23
1/28	4.042e−04	6.241e−04	4.20	4.11
1/56	9.691e−05	1.523e−04	–	–
1/112	2.369e−05	3.758e−05	–	–

Simulations in 1-D and 2-D

In Fig. 1 numerical solutions of $\left(\mathrm{P}_1^{h,\Delta t}\right)$ are plotted in 1-D with Kinetics (i) (see figure caption for parameter values and initial data). Initial data are small spatial perturbations of the stationary solutions of the corresponding ODE system. As α is varied from 0.5 to 0.05 we see the four basic 1-D solutions types, namely (a) stationary, (b) smooth oscillatory, (c) intermittent 'chaos', and (d) 'chaos' covering (most of) the domain. In Fig. 1c we used the same initial data and parameter values as in [38]. However, the paper [38] does not state the mesh and temporal discretisation parameters, or the numerical method employed. Our results are qualitatively similar, with the same intermittent spatial structures appearing at roughly the same positions.

In Fig. 2 the approximate prey densities U^n for scheme $\left(\mathrm{P}_1^{h,\Delta t}\right)$ are plotted using Kinetics (i) in (a)–(c) and Kinetics (ii) in (d). The figures represent snapshots at various

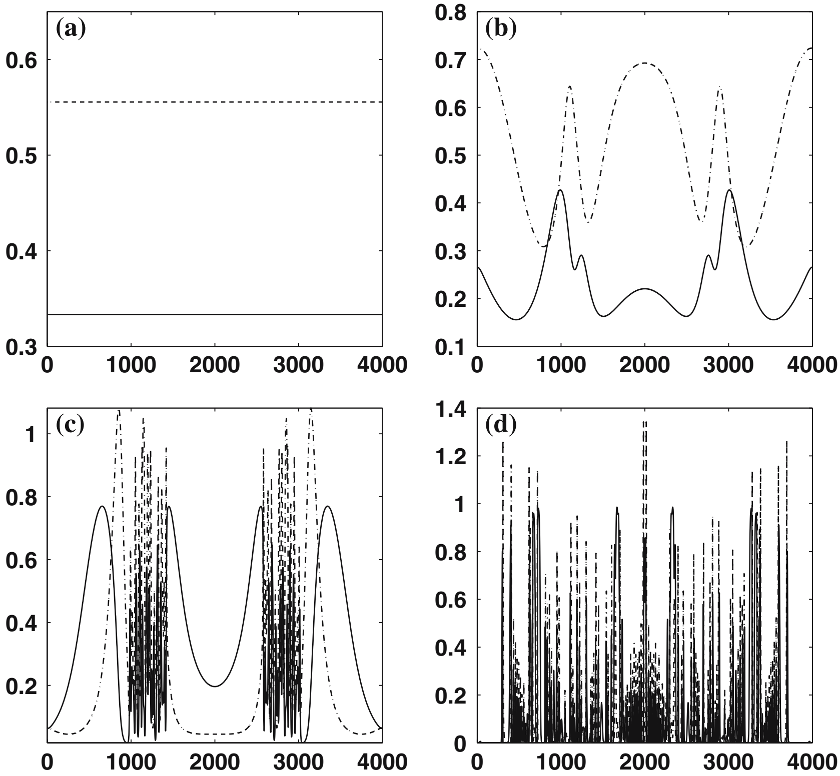

Fig. 1 1-D numerical solutions of $\left(\mathbf{P}_1^{h,\Delta t}\right)$ with Kinetics (i); *solid lines* for prey U^n and *dashed lines* for predators V^n. Parameter values and initial data: $\beta = 2$, $\gamma = 4/5$, $\delta = 1$, $T = 600$, $h = 1$, $\Delta t = 10^{-4}$, $T = 600$, $U^0 = \pi^h\{u^* + 10^{-8}(x-1200)(x-2800)\}$, $V^0 = v^*$. **a** $\alpha = 1/2$ ($u^* = 1/3$, $v^* = 5/9$), **b** $\alpha = 33/80$ ($u^* = 11/40$, $v^* = 319/640$), **c** $\alpha = 3/10$, ($u^* = 1/5$, $v^* = 2/5$), **d** $\alpha = 1/20$, ($u^* = 1/30$, $v^* = 29/360$)

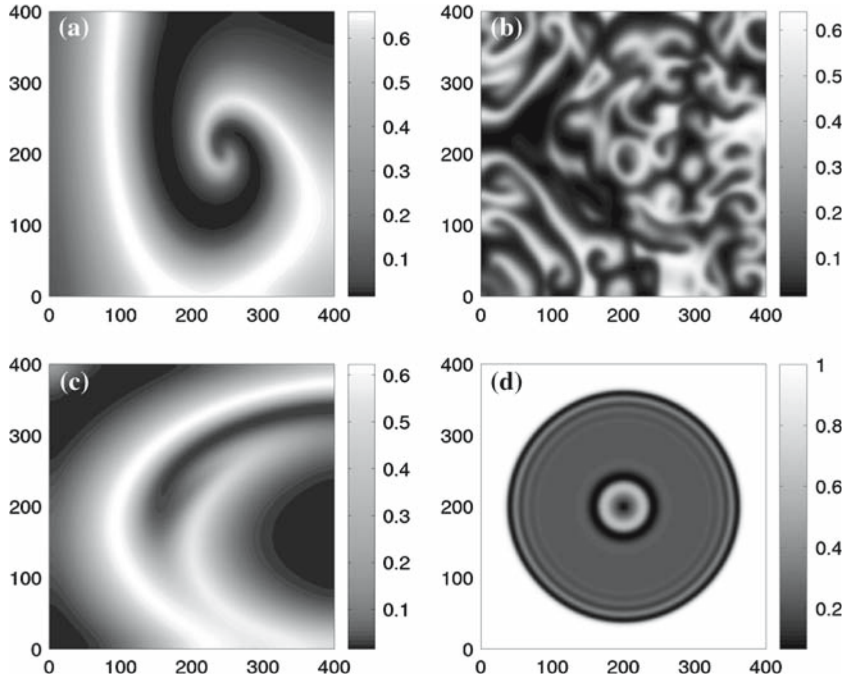

Fig. 2 Snapshots of approximate prey densities U^n for $\left(P_1^{h,\Delta t}\right)$ with Kinetics (i) in (a)–(c), and Kinetics (ii) in (d). In all plots $h = 1$, $\Delta t = 1/384$, $\delta = 1$. Parameter values and initial data at **a** $T = 150$, and **b** at $T = 1000$: $\alpha = 0.4$, $\beta = 2.0$, $\gamma = 0.6$, $U^0 = \pi^h\{6/35 - 2\times 10^{-7}(x - 0.1y - 225)(x - 0.1y - 675)\}$, $V^0 = \pi^h\{116/245 - 3\times 10^{-5}(x - 450) - 1.2\times 10^{-4}(y - 150)\}$. Parameter values and initial data for **c** at $T = 120$: $\alpha = 0.4$, $\beta = 2.0$, $\gamma = 0.6$, $U^0 = \pi^h\{6/35 - 2\times 10^{-7}(x - 180)(x - 720) - 6\times 10^{-7}(y - 90)(y - 210)\}$, and $V^0 = \pi^h\{116/245 - 3\times 10^{-5}(x - 450) - 6\times 10^{-5}(y - 135)\}$. Parameter values and initial data for **d** at $T = 110$: $\alpha = 1.5$, $\beta = 1.0$, $\gamma = 5.0$, $U^0 = 1.0$, $V^0 = 0.2$ if $(x - 200)^2 + (y - 200)^2 < 400$ and zero otherwise

times T in the domain $\Omega = [0, 400]^2$ (for the parameter values and initial data see the caption). Figure 2a–c correspond to Figs. 10a, 10f, and 11b, respectively, in [38]. We used the same parameter values and initial conditions as in [38]. However, the paper [38] does not state the mesh and temporal discretisation parameters, or the numerical method employed. Our plots are qualitatively similar, with a spiral wave clearly visible in Fig. 2a, and irregular patchy structures in Fig. 2b. The main difference between our results and those in [38] is that in Fig. 11b spiral waves are present, while in Fig. 2c they are absent. This suggests that the spiral waves in Fig. 11b are spurious. In Fig. 2d the initial localised introduction of predators into a homogeneous distribution of prey led to the invasion of predators into the domain over time, with perfectly circular bands of regular spatiotemporal oscillations behind the wavefront. We used the same parameter values as in [54], but the precise initial conditions are not given. The results are qualitatively similar. Due to the 'chaotic' solutions in Fig. 2b we were unable to achieve exact agreement between the approximations of $\left(P_1^{h,\Delta t}\right)$ and $\left(P_2^{h,\Delta t}\right)$ in this case.

5 Conclusions

We studied two semi implicit, fully discrete, piecewise linear finite element methods for approximating the solutions of nonlinear reaction–diffusion systems modelling predator–prey interactions with the Holling type II functional response and logistic growth of the prey. After rigorously analysing a semi discrete, piecewise linear finite element method (with mass lumping), we proved fully discrete estimates and a fully discrete error bound with respect to the $L^\infty(0, T; L^2(\Omega))$ and $L^2(0, T; H^1(\Omega))$ norms, with rate of convergence $\mathcal{O}(h + \Delta t^{1/2})$. Numerical results indicate that the rate of convergence is $\mathcal{O}(h + \Delta t)$ (at least in 1-D), which is consistent with the application of the Backward Euler method applied to the heat equation. The fully discrete finite element scheme is easy to implement, and the resulting linear systems readily solved with well-known direct or iterative solvers.

In 1-D we showed how modest changes in a single parameter of the system, namely α, can lead to dramatic changes in the qualitative dynamics of solutions. In contrast, the experiments in [38] focused on how the solution dynamics depended on the choice of initial conditions. In 2-D there is a lack of reproducible numerical results in the literature for the generic predator–prey systems studied in this paper, and thus our results are useful for future comparative work.

The results of this paper contribute to the important task of putting the numerical analysis community in contact with interesting problems coming from biology.

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