Implicit–explicit timestepping with finite element approximation of reaction–diffusion systems on evolving domains

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ABSTRACT. We present and analyse an implicit–explicit timestepping procedure with finite element spatial approximation for a semilinear reaction–diffusion systems on evolving domains arising from biological models, such as Schnakenberg’s (1979). We employ a Lagrangian formulation of the model equations which permits the error analysis for parabolic equations on a fixed domain but introduces technical difficulties, foremost the space-time dependent conductivity and diffusion. We prove optimal-order error estimates in the $L_\infty(0,T;L^2(\Omega))$ and $L^2(0,T;H^1(\Omega))$ norms, and a pointwise stability result. We remark that these apply to Eulerian solutions. Details on the implementation of the Lagrangian and the Eulerian scheme are provided. We finally report on numerical experiments for an application to pattern formation on evolving domains, where we observe novel complex pattern transitions in multicomponent systems and the emergence of patterns with different wavelengths under nonuniform evolution.

1. INTRODUCTION

Since the seminal paper of Turing [29], time-dependent reaction–diffusion systems (RDSs) have been studied as models of pattern formation in natural-process driven morphogenesis and developmental biology (see Murray [22] for details). An important generalisation of these models consists in considering RDSs posed on evolving domains. This stems from the now relatively well-known observation that in many cases growth of organisms plays a pivotal role in the emergence of patterns and their evolution during growth development [13, 22].

RDSs on evolving domains have also a wider scope of application, such as competing-species of micro-organisms in environmental biology, chemistry of materials and corrosion processes, the spread of pollutants, etc. Numerical simulations of RDSs on growing, or more generally time-evolving, domains reproducing empirically observed pattern formation processes are commonly used [2, 3, 7, 13, 21]. It is essential for scientists to computationally approximate and appreciate the error between simulations and exact solutions of such RDSs. Galerkin finite elements [28] are among the methods of choice to approximate such systems.

In spite of their widespread use, to the best of our knowledge, no complete error analysis of approximating finite element schemes for nonlinear reaction–diffusion systems on evolving domains is available in the literature, thus motivating this work. This is a sibling paper to [30] where we analysed the well-posed nature of (exact) RDSs on evolving domains. In most practical applications, the evolving domain is usually a surface embedded in the three-dimensional Euclidean space, but for simplicity we restrict our discussion to the case where both the reference domain and the evolving domain are flat, deferring thus the analysis of RDSs on evolving curved surfaces.

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1.1. Problem (RDS on a time-dependent evolving domain). We study a RDS, also considered in [6, 17], which models a system of chemicals that interact through the reaction terms only and diffuse in the domain independently of each other. Given an integer \( m \geq 1 \), the vector \( u(x,t) \in \mathbb{R}^m \), denoting the concentration of the chemical species \( i = 1, \ldots, m \), at a spatial point \( x \in \Omega_t \subset \mathbb{R}^d \), \( d = 1, 2, 3 \), at time \( t \in [0, T] \), \( T > 0 \), satisfies the following initial–boundary value problem

\[
\begin{align*}
\partial_t u_i(x,t) - D_i \Delta u_i(x,t) + \nabla \cdot [a u_i] (x,t) &= f_i (u(x,t)) , & x \in \Omega_t, t \in (0, T], \\
\nu \cdot \nabla u_i(x,t) &= 0, & x \in \partial \Omega_t, t > 0, \\
u_i(x,0) &= u_i^0(x), & x \in \Omega_0,
\end{align*}
\]

(1.1)

where \( \Omega_t \), detailed in [2, 22], is a simply connected Lipschitz continuously evolving domain with respect to \( t \in [0, T] \), and \( D := (D_1, \ldots, D_m)^T \) is a vector of strictly positive diffusion coefficients. Detailed assumptions on the nonlinear reaction vector field \( f := (f_1, \ldots, f_m)^T \) are given in [2, 5]. The convection \( a = (a_1, \ldots, a_d)^T \) is induced by the material deformation due to the evolution of the domain. The initial data \( u^0 \) is a positive-entry bounded field. Since we are primarily interested in pattern formation phenomena that arise as a result of self-organisation within a domain without outside-world communication we consider homogeneous Neumann boundary conditions, but other types of boundary conditions could be studied as well within our framework.

1.2. Main results. The core result in this paper is Theorem 5.1 where we prove optimal convergence rates of the discrete solution in \( L_\infty (0, T; L_2(\hat{\Omega}))^m \) and \( L_2(0, T; H^1(\hat{\Omega}))^m \) (where \( \hat{\Omega} \) is a transformed version of \( \Omega_t \) to be described next). Our theoretical results are illustrated by numerical experiments, aimed mainly at quantifying the pattern formation phenomena related to the type of growth in the domains. The results of numerical experiments exhibit the emergence of complex patterns when multispecies RDSs are considered as well as patterns of different wavelengths when nonuniform domain evolution is considered. To the best of our knowledge, this article is the first to expose such results.

1.3. A Lagrangian approach. We employ, both for the analysis and the implementation of the computational method, a Lagrangian formulation of Problem [17] in the sense employed in fluid-dynamics, i.e., where the evolving domain, \( \Omega_t \subset \mathbb{R}^d \), is the image of a time-dependent family of diffeomorphisms \( A_t \) on a reference domain \( \hat{\Omega} \subset \mathbb{R}^d \). The \( m \) parabolic equations with constant diffusion coefficient constituting the RDS on \( \Omega_t \) are thus pulled-back into equations on a fixed domain, albeit with space-time dependent coefficients. The fixed domain setting permits us to use the standard Bochner space machinery needed for evolution equations of parabolic type. On the other hand, we are thus left to deal (computationally and analytically) with three interacting difficulties: (1) \( m \) coupled equations, (2) the nature of the nonlinearity \( f \) coupling the equations, (3) the non-constant diffusion and velocity coefficients, especially as functions of time. Our approach in tackling the nonlinearity consists in constructing a suitable globally Lipschitz extension of the nonlinear reaction field that coincides with it in a neighbourhood of the exact solution and then proving that both the exact solution and the numerical solution are confined to the domain of the original (non-extended) nonlinearity. We use mainly parabolic energy techniques, but must have some pointwise control in order to bound the nonlinearities.

Although all our error estimates are derived for the Lagrangian formulation, given that the domain evolution is prescribed, they carry in a straightforward manner to the Eulerian framework. The situation would be more delicate if the domain evolution was itself an unknown as a geometric motion coupled with the RDS, but this is outside the scope of this study.

1.4. Implicit-explicit schemes. The fully discrete method that we analyse, is a fully practical method, implemented in the ALBERTA toolbox (code available upon request), using an implicit-explicit backward Euler scheme to derive the time-discretization [13]. On fixed domains, Zhang et al. [32] analyse a second order implicit-explicit finite element scheme for the Gray-Scott model and Garvie and Trenchea [9] analyse a first order scheme for an RDS that models predator prey dynamics. Recently Mackenzie
and Madzvamuse [16] analysed a finite difference scheme approximating the solution of a linear RDS on a domain with continuous spatially linear isotropic evolution. Our study is novel, in that, we propose and analyse a finite element method to approximate RDSs on a domain with continuous (possibly nonlinear) evolution. This creates a space-time-dependent coefficients impacting the diffusion and the time-derivative term which complicates the fully discrete scheme’s analysis and requires a careful treatment of the timestep, depending on the rate of domain evolution. In spite of it being only first order in time, the proposed implicit-explicit method is robust for the applications we have in mind, where long time integration is essential and the problems are often posed on complex geometries such as the surface of an organism.

1.5. Outline. The structure of this paper is as follows: in §2 we introduce the notation employed throughout this article, we state our model problem together with the assumptions that we make on the problem data and the domain evolution. We present the weak formulation of the continuous problem and define a modified nonlinear reaction function which we introduce for the analysis. In §3 we present the semidiscrete (space-discrete) and the fully discrete finite element schemes with some remarks regarding implementation, allowing the practically minded reader to skip over the analysis through to §6. We then analyse the semidiscrete scheme in §4 and the fully discrete scheme in §5 proving optimal rate error bounds as well as a maximum-norm stability result, whereby the stabilising effect of domain growth observed in the continuous case is preserved at the discrete level and in the numerical schemes. In §6 we provide two concrete implementations (Eulerian and Lagrangian) of the finite element scheme with a set of reaction kinetics commonly encountered in developmental biology, considering domains with spatially linear and nonlinear evolution. In §7 we present computational experiments to illustrate our theoretical results and to study as of yet unexplored solution behaviour exhibited by RDSs on evolving domains in two-space dimensions.

2. Notation and Setup

In this section we define most of the basic notation for the rest of the paper, introduce the evolving domain framework, set the detailed blanket assumptions and introduce a pulled-back version of Problem 1.1.

2.1. Calculus and function spaces. Given an open and bounded stationary domain \( \Pi \subset \mathbb{R}^d \) and a function \( \eta \in C^1(\Pi; \mathbb{R}^m) \), we define the Jacobian matrix of \( \eta \)
\[
\nabla \eta(x) := \begin{bmatrix}
\partial_{x_1} \eta_1(x) & \cdots & \partial_{x_1} \eta_m(x) \\
\vdots & \ddots & \vdots \\
\partial_{x_d} \eta_1(x) & \cdots & \partial_{x_d} \eta_m(x)
\end{bmatrix}, \quad \text{for } x \in \Pi,
\]
and the divergence of \( \eta \)
\[
\nabla \cdot \eta(x) := \sum_{i=1}^d \partial_{x_i} \eta_i(x).
\]
For the case of a scalar-valued function \( \eta \in C^1(\Pi; \mathbb{R}) \), we define the Laplacian of \( \eta \)
\[
\Delta \eta(x) := \sum_{i=1}^d \partial_{x_i x_i} \eta(x).
\]
In an effort to compress notation for spatial derivatives, we introduce the convention used above, that if the variable with respect to which we differentiate is omitted, it should be understood as the spatial argument of the function.
We denote by $L^p (\Pi)$, $W^{p,k} (\Pi)$ and $H^k (\Pi)$ the Lebesgue, Sobolev and Hilbert spaces respectively, as defined by the following: for measurable $\eta$ and for $p, k \in [1, \infty)\nolimits$

\begin{equation}
L^p (\Pi) := \left\{ \eta : \int_\Pi |\eta|^p < \infty \right\},
\end{equation}

\begin{equation}
L_\infty (\Pi) := \left\{ \eta : \sup_{x \in \Pi} |\eta(x)| < \infty \right\},
\end{equation}

\begin{equation}
W^{k,p} (\Pi) := \left\{ \eta \in L^p (\Pi) : \sum_{\alpha \leq k} \nabla^\alpha \eta \in L^p (\Pi) \right\},
\end{equation}

\begin{equation}
H^k (\Pi) := W^{2,k} (\Pi).
\end{equation}

For measurable functions $\eta, \mu : \Pi \to \mathbb{R}$, we introduce the following notation

\begin{equation}
\langle \eta, \mu \rangle_\Pi := \int_\Pi \eta(x)\mu(x) \, dx,
\end{equation}

\begin{equation}
\|\eta\|_{L^2 (\Pi)} := \langle \eta, \eta \rangle_\Pi^{1/2},
\end{equation}

\begin{equation}
|\eta|_{H^k (\Pi)} := |\nabla^k \eta|_{L^2 (\Pi)}, \quad \text{for } k \in \mathbb{Z}_+,\n\end{equation}

\begin{equation}
\|\eta\|_{H^k (\Pi)} := \left( \|\eta\|^2_{L^2 (\Pi)} + \sum_{j=1}^k \|\nabla^j \eta\|^2_{L^2 (\Pi)} \right)^{1/2}.
\end{equation}

For vector valued functions $\eta, \mu : \Pi \to \mathbb{R}^m$, we denote

\begin{equation}
\langle \eta, \mu \rangle_{\Pi,m} := \sum_{i=1}^m \int_\Pi \eta_i(x)\mu_i(x) \, dx,
\end{equation}

with the corresponding modifications to the norms and seminorms.

\section*{2.2. Evolving domain.}

Let $\hat{\Omega} \subset \mathbb{R}^d$ be a simply connected domain with Lipschitz boundary; we will call it the reference domain. We define the evolving domain as a time-parametrised family of domains

\begin{equation}
\{\Omega_t := \mathcal{A}_t(\hat{\Omega})\}_{0 \leq t \leq T} \quad \text{where } \mathcal{A}_t : \hat{\Omega} \to \Omega_t \text{ is a } C^1 \text{-diffeomorphism for each fixed } t \in [0, T].
\end{equation}

The Jacobian matrix of $\mathcal{A}_t(\cdot)$, its determinant and inverse will be respectively denoted by

\begin{equation}
J_t(\xi) := \nabla \mathcal{A}_t(\xi), \quad J_t^{-1}(\xi) := \det J_t(\xi) \quad \text{and } K_t(\xi) := (\nabla \mathcal{A}_t(\xi))^{-1} \text{ for each } (\xi, t) \in \hat{\Omega} \times [0, T].
\end{equation}

We will use also the evolution induced convection on the evolving domain

\begin{equation}
a(x, t) := \partial_t \mathcal{A}_t(\mathcal{A}_t^{-1}(x)) \text{ for } x \in \Omega_t \text{ and } t \in [0, T].\n\end{equation}

From classical results \cite{1} we have the following expression

\begin{equation}
\partial_t J(\xi, t) = J_t(\xi) \nabla \cdot a(\mathcal{A}_t(\xi), t) \text{ for } (\xi, t) \in \hat{\Omega} \times [0, T].
\end{equation}

To aid the exposition we define $\mathcal{Q}$ to be the topologically cylindrical space-time domain:

\begin{equation}
\mathcal{Q} := \{(x, t) : x \in \Omega_t, t \in [0, T]\}.
\end{equation}

We now introduce notation to relate functions defined on the evolving domain to functions defined on the reference domain. Given a function $g : \mathcal{Q} \to \mathbb{R}$ we denote by $\hat{g} : \hat{\Omega} \times [0, T] \to \mathbb{R}$ its pullback on the reference domain, defined by the following relationship

\begin{equation}
\hat{g}(\xi, t) := g(\mathcal{A}_t(\xi), t) \text{ for } (\xi, t) \in \hat{\Omega} \times [0, T].
\end{equation}
Assuming sufficient smoothness on the function \( g \), using (2.18) and the chain rule we may relate time-
differentiation on the reference and evolving domains\(^1\)
\[
(2.19) \quad \partial_t \hat{g}(\xi, t) = \partial g \left( A_\ell(\xi), t \right) + [a \cdot \nabla g] \left( A_\ell(\xi), t \right), \quad (\xi, t) \in \hat{\Omega} \times [0, T].
\]
The right hand side of (2.19) is commonly known as the material derivative of \( g \) with respect to the
velocity \( a \). The following result relates the norm of a function \( g : Q \to \mathbb{R} \) on the evolving domain with its
pullback \( \hat{g} \) on the reference domain:
\[
(2.20) \quad \|g\|_{L^2(\Omega)}^2 = \langle J \hat{g}, \hat{g} \rangle_{\hat{\Omega}} =: \|\hat{g}\|_{\hat{\Omega}}^2.
\]
For the gradient of a sufficiently smooth function \( g : Q \to \mathbb{R} \), we have
\[
(2.21) \quad \|\nabla g\|_{L^2(\Omega)}^2 = \langle J_\ell K \hat{\nabla} \hat{g}, K \hat{\nabla} \hat{g} \rangle_{\hat{\Omega}} = \langle B \hat{\nabla} \hat{g}, \hat{\nabla} \hat{g} \rangle_{\hat{\Omega}} =: \|\hat{g}\|_{B, \ell}^2,
\]
where \( B := JK^T \). For \( t \in [0, T] \) we define the bilinear form
\[
(2.22) \quad b_t(\hat{v}, \hat{w}) := \langle B, \hat{\nabla} \hat{v}, \hat{\nabla} \hat{w} \rangle_{\hat{\Omega}} \text{ for } \hat{v}, \hat{w} \in H^1(\hat{\Omega}).
\]
Assumption 2.3 implies that there exist \( \mu, \bar{\mu} \in \mathbb{R}_+ \) such that for \( i = 1, \ldots, m \) and all \( \hat{v} \in H^1(\hat{\Omega}) \),
\[
(2.23) \quad \mu \|\nabla \hat{v}\|_{L^2(\hat{\Omega})}^2 \leq b_t(\hat{v}, \hat{v}) \leq \|B\|_{L^\infty(\hat{\Omega})} \|\nabla \hat{v}\|_{L^2(\hat{\Omega})}^2 = \bar{\mu} \|\nabla \hat{v}\|_{L^2(\hat{\Omega})}^2.
\]

2.3. **Assumption (Regularity of the mapping)**. We assume the following regularity on the mapping \( A \)
between the reference domain \( \hat{\Omega} \) and the evolving domain \( \Omega_t : \)
\[
(2.24) \quad A \in C^k(\hat{\Omega} \times [0, T]) \quad \text{and} \quad A_{\ell} \in C^k(\hat{\Omega}) \text{ for } t \in [0, T],
\]
where \( k \) will be taken equal to the degree of the basis functions of the finite element space defined in the
following section. To ensure the mapping is invertible we assume the determinant of the Jacobian \( J \) of
the mapping \( A \) (cf. (2.14)) satisfies
\[
(2.25) \quad J > 0 \text{ in } \hat{\Omega} \times [0, T].
\]

2.4. **The RDS reformulated on the reference domain**. Using (2.18)–(2.21) and a change of variable
in the divergence, we obtain the following equivalent formulation of Problem 1.1 on a reference domain.
Denote by \( \tilde{u} : \hat{\Omega} \times [0, T] \to \mathbb{R}^m \) the function that satisfies for \( i = 1, \ldots, m, \)
\[
(2.26) \quad \partial_t \tilde{u}_i - \frac{D_i}{J} \nabla \cdot (B \nabla \tilde{u}_i) + \hat{u}_i \nabla \cdot \hat{a} = f_i(\tilde{u}), \quad \text{on } \hat{\Omega} \times (0, T],
\]
\[
\hat{v} \cdot B \nabla \tilde{u}_i = 0, \quad \text{on } \partial \hat{\Omega} \times (0, T],
\]
\[
\tilde{u}_i(\xi, 0) = \tilde{u}_i^0(\xi), \quad \xi \in \hat{\Omega}.
\]
where
\[
(2.27) \quad \hat{a}(\xi, t) = \partial_t A_{\ell}(\xi) \text{ for } (\xi, t) \in \hat{\Omega} \times [0, T].
\]

2.5. **Assumption (Nonlinear reaction vector field)**. We assume throughout that \( f \) is of the form
\[
(2.28) \quad f_i(z) = z_i F_i(z), \quad \text{for all } z \in \text{Dom } f := I \text{ and each } i = 1, \ldots, m,
\]
for some vector field \( F \in C^1(I) \). As a result \( f \in C^1(I) \) and it is locally Lipschitz.

2.6. **Assumption (Existence and regularity)**. We assume the global existence of a solution \( \tilde{u} \) to Problem 2.4
Furthermore we assume \( \tilde{u} \) is in \( H^{\ell+1}(\hat{\Omega})^m \) with \( \partial_{\ell} \tilde{u} \) in \( H^{\ell+1}(\hat{\Omega})^m \) where \( \ell \) is the polynomial
degree of the finite element space defined in the following section.

\(^1\) When confusion may arise, such as in (2.19) for a positive integer \( i, \partial_i f \) denotes the partial derivative with respect to the \( i \)-th
argument of the function \( f \). When there is no risk of confusion we write \( \partial_i f \) for the time derivative of a time-dependent function \( f \)
even when such a variable is not explicitly written in the arguments.
The function $I$

### Section 3.1: Spatial discretisation set-up.

Discussing some properties of the semidiscrete scheme and then passing to the fully discrete scheme. This end, we define $\hat{u}$ into separate steps. For the spatial approximation, we employ a conforming finite element method. To purposes of our analysis we introduce a modified principle [28, pg. 83] means we cannot guarantee the discrete solution remains in the region $I_\delta := \prod_{i=1}^d [u_i^-, u_i^+]$ with $u^- > 0$ and assumption 2.5 holds with the region $I_\delta := \prod_{i=1}^d [u_i^- - \delta, u_i^+ + \delta]$ a subset of $\mathbb{R}_+^m$.

### Section 2.8: Weak formulation.

For the purposes of constructing a finite element discretisation, we introduce a weak formulation associated with Problem 2.4. The problem is to find $\hat{u}_i \in L_2 (0, T; H^1 (\Omega))$ with $\partial_t \hat{u}_i \in L_2 (0, T; H^{-1} (\Omega))$ such that

\begin{equation}
(2.29)
\langle J \left( \partial_t \hat{u}_i + \hat{u}_i \nabla \cdot (A_i (\xi), t) \right), \hat{\xi} \rangle + D_i b_t (\nabla \hat{u}_i, \nabla \hat{\xi}) = \langle J f_i (\hat{u}), \hat{\xi} \rangle_{\Omega},
\end{equation}

for all $\hat{\xi} \in H^1 (\Omega)$. Using the expression for the time-derivative of the determinant of the Jacobian (2.16), we have

\begin{equation}
(2.30)
\langle \partial_t (J \hat{u}_i), \hat{\xi} \rangle_{\Omega} + D_i b_t (\nabla \hat{u}_i, \nabla \hat{\xi}) = \langle J f_i (\hat{u}), \hat{\xi} \rangle_{\Omega}, \quad \forall \hat{\xi} \in H^1 (\Omega).
\end{equation}

We shall use (2.30) to construct a finite element scheme to approximate the solution to Problem 1.1 on the reference domain. In [6] we illustrate that the resulting scheme may be solved both on the reference (Lagrangian scheme) or the evolving (Eulerian scheme) domain.

### Section 2.9: Extended nonlinear reaction function.

In general the techniques used to show Assumptions 2.5 and 2.6 hold utilise the maximum principle [27, 30]. In the discrete case, the absence of a maximum principle [28, pg. 83] means we cannot guarantee the discrete solution remains in the region $I_\delta$. For the purposes of our analysis we introduce a modified globally Lipschitz nonlinear reaction function. Recalling $I_\delta$ and $F$ from Assumption 2.5 we define $\tilde{F} \in C^1 (\mathbb{R}^m)$ such that

\begin{equation}
(2.31)
\begin{cases}
\tilde{F}(z) = F(z), & \text{for } z \in I_\delta, \\
\tilde{F}'(z) < C, & \text{for } z \in \mathbb{R}^m,
\end{cases}
\end{equation}

\begin{align}
&f_i (z) := z_i \tilde{F}'(z), \quad \text{for } z \in \mathbb{R}^m. \\
&(2.32) f(u) = f(u).
\end{align}

Thus, we may without restriction replace $f$ with $\tilde{f}$ in (1.1).

### Section 3. Finite element method

In this section we design the finite element method, first by discretising Problem 2.4 in space only, discussing some properties of the semidiscrete scheme and then passing to the fully discrete scheme.

#### 3.1: Spatial discretisation set-up.

We shall split the spatial and temporal discretisation of Problem 1.1 into separate steps. For the spatial approximation, we employ a conforming finite element method. To this end, we define $\mathcal{T}$ a triangulation of the reference domain. We shall consistently denote by $\hat{h} := \max_{s \in \mathcal{T}} \text{diam}(s)$ the mesh-size of $\mathcal{T}$. We assume the triangulation $\mathcal{T}$ fulfills the following properties:

- By $s \in \mathcal{T}$ we mean $s$ is an open simplex (interval, triangle or tetrahedron for $d = 1, 2$ or 3 respectively).
- $\mathcal{T}$ is conforming, i.e., for any $s, k \in \mathcal{T}$, $\bar{s} \cap \bar{k}$ is either $\emptyset$, a vertex, an edge or a face common to $s$ and $k$ or the full simplex $\bar{s} = \bar{k}$.
- No error due to boundary approximation, i.e., $\cup_{s \in \mathcal{T}} \bar{s} = \bar{\Omega}$ (we make this assumption for ease of exposition and it may be relaxed depending on the application).
For a sequence \( \{ \hat{\mathcal{T}}_i \}_{i=1}^{\infty} \) of conforming triangulations, we assume the \textit{quasi-uniformity} of the sequence holds, i.e., there exist \( C_1, C_2 \) independent of \( i \) such that

\[
C_1 \hat{h} \leq \hat{h}_s \leq C_2 \hat{h}_s^2, \quad \text{for all } s \in \hat{\mathcal{T}}_i, i = 1, 2, \ldots,
\]

where \( \hat{h}_s \) and \( \hat{h}_s \) are the radius of the largest ball contained in \( s \) and the diameter of \( s \) respectively. Furthermore we note that our assumption of quasi-uniformity implies that the family of triangulations is shape-regular \cite{26} pg. 159).

Given the triangulation \( \hat{\mathcal{T}} \), we now define a finite element space on the reference configuration:

\[
\hat{V} := \left\{ \hat{\Phi} \in H^1(\hat{\Omega}) : \hat{\Phi}|_s \text{ is piecewise polynomial of degree } \ell \right\}.
\]

We utilise the following known results about the accuracy of the finite element space \( \hat{V} \). By the definition of \( \hat{V} \), we have for \( \hat{v} \in H^{\ell+1}(\hat{\Omega}) \) (see for example Brenner and Scott \cite{4} or Thomée \cite{28}),

\[
\inf_{\hat{\Phi} \in \hat{V}} \left\{ \| \hat{v} - \hat{\Phi} \|_{L^2(\hat{\Omega})} + \| \hat{v} - \hat{\Phi} \|_{L^2(\hat{\Omega})} \right\} \leq C\hat{h}^{\ell+1} \| \hat{v} \|_{H^{\ell+1}(\hat{\Omega})}.
\]

In the analysis we shall make use of the fact that \(3.3\) is satisfied by taking the Lagrange interpolator \( \Lambda^h : H^{\ell+1}(\hat{\Omega}) \to \hat{V} \) in place of \( \hat{\Phi} \). Let \( \hat{T}^h : \hat{C}^0 \to \hat{V} \) be a Clement type interpolant \( \hat{\Phi}^0 \) and \( \ell + 1 > \frac{d}{2} \), where \( d \) is the spatial dimension. The following bound holds

\[
\| \hat{v} - \hat{T}^h \hat{v} \|_{L^2(\hat{\Omega})} \leq C\hat{h}^{\ell+1-d/2} \| \hat{v} \|_{H^{\ell+1}(\hat{\Omega})}.
\]

We shall make use of the following inverse estimate valid on quasiuniform sequences of triangulations:

\[
\| \hat{\Phi} \|_{L^2(\hat{\Omega})} \leq C\hat{h}^{-d/2} \| \hat{\Phi} \|_{L^2(\hat{\Omega})} \quad \forall \hat{\Phi} \in \hat{V}.
\]

3.2. \textbf{Semidiscrete approximation.} We define the spatially semidiscrete approximation of the solution of Problem \ref{1.1} to be a function \( \hat{u}^h : [0, T] \to \hat{V} \), such that for \( i = 1, \ldots, m \),

\[
\left\{ \begin{aligned}
&\left\langle \partial_t (J \hat{u}^h_i), \hat{\Phi} \right\rangle_{\hat{\Omega}} + \left\langle D_i B \nabla \hat{u}^h_i, \nabla \hat{\Phi} \right\rangle_{\hat{\Omega}} = \left\langle J \hat{f}_i (\hat{u}^h_i), \hat{\Phi} \right\rangle_{\hat{\Omega}}, \quad \forall \hat{\Phi} \in \hat{V}, \\
&\hat{u}^h_i (0) = \Lambda^h \hat{u}^h_i^0,
\end{aligned} \right.
\]

where \( \Lambda^h \) is the Lagrange interpolant.

3.3. \textbf{Proposition (Solvability of the semidiscrete scheme).} Let Assumptions \ref{2.6} and \ref{2.3} hold. Then, the semidiscrete scheme \(3.6\) possesses a unique solution \( \hat{u}^h \in L^\infty (0, T)^m \).

\textbf{Proof.} In \(3.6\) if we write \( \hat{u}^h_i(t) \) as \( \sum_{j=1}^{\dim(\hat{V})} \alpha_j \hat{\Phi}_j \), we obtain a system of \( \dim(\hat{V}) \) ordinary differential equations for each \( i \). By assumption the initial data for each ODE is bounded. From Assumption \ref{2.3} and the construction of \( \hat{f} \) \ref{2.31}, we have that \( J, \hat{f} \) and their product are continuous globally Lipschitz functions. From ODE theory (for example \cite{24}) we conclude that \(3.6\) possesses a unique bounded solution. \( \square \)

3.4. \textbf{The effect of domain evolution on the semidiscrete solution.} We now examine the stability of \(3.6\) and show that domain growth has a \textit{diluting} or \textit{stabilising} effect on the semidiscrete solution, mirroring results for the continuous problem \cite{14}. Taking \( \Phi = \hat{u}^h \) in \(3.6\) gives for \( i = 1, \ldots, m \),

\[
\left\langle \partial_t (J \hat{u}^h_i), \hat{u}^h_i \right\rangle_{\hat{\Omega}} + D_i b_i \left( \nabla \hat{u}^h_i, \nabla \hat{u}^h \right)_{\hat{\Omega}} = \left\langle J \hat{f}_i (\hat{u}^h_i), \hat{u}^h_i \right\rangle_{\hat{\Omega}}.
\]

For the first term on the left of \(3.7\) we have

\[
\left\langle \partial_t (J \hat{u}^h_i), \hat{u}^h_i \right\rangle_{\hat{\Omega}} = \frac{d}{dt} \left\langle J \hat{u}^h_i, \hat{u}^h_i \right\rangle_{\hat{\Omega}} - \left\langle J \hat{u}^h_i, \partial_t \hat{u}^h_i \right\rangle_{\hat{\Omega}}.
\]
Application of Reynold’s transport theorem \([11]\) gives
\[
(3.9) \quad \left\langle \partial_t (J \dot{u}^h), \dot{u}^h \right\rangle_{\Omega} = \frac{1}{2} \left( \frac{d}{dt} \| \dot{u}^h \|^2_{J} + \left\langle J \dot{u}^h, a(\mathcal{A}(\xi), t) \right\rangle_{\Omega} \right).
\]
Now dealing with the right hand side of (3.7), using (2.31) and the mean-value theorem (MVT) we have with \(\bar{C}\) from (2.31)
\[
\left| \tilde{f}_i(u^h) \right| \leq \left| \tilde{f}_i(0) \right| + \left| \tilde{f}_i(u^h) - \tilde{f}_i(0) \right|
\]
\[
(3.10) \quad \leq \tilde{f}_i(0) + \bar{C} \sum_{j=1}^{m} |\tilde{u}^h_j|.
\]
Therefore we have
\[
(3.11) \quad \left| \left\langle J \tilde{f}_i(u^h), \dot{u}^h_i \right\rangle_{\Omega} \right| \leq \bar{C} \left| \left\langle J \sum_{j=1}^{m} |\tilde{u}^h_j|, \dot{u}^h_i \right\rangle_{\Omega} + \left| \left\langle J \tilde{f}_i(0), \dot{u}^h_i \right\rangle_{\Omega} \right| \right|.
\]
Applying Young’s inequality gives
\[
(3.12) \quad \left| \left| \left\langle J \tilde{f}_i(u^h), \dot{u}^h_i \right\rangle \right| \right| \leq \bar{C} \left( \frac{1}{2} \sum_{j \neq i} |\tilde{u}^h_j|^2 + \frac{m + 1}{2} \| \dot{u}^h_i \|^2 \right)
\]
\[
+ \frac{1}{2} \| \dot{u}^h_i \|^2 + \bar{C} \tilde{f}_i(0),
\]
where \(\bar{C} \tilde{f}_i(0) \in \mathbb{R}^+\) depends on \(\tilde{f}_i(0)\). Summing over \(i\) we have
\[
(3.13) \quad \sum_{i=1}^{m} \left| \left\langle J \tilde{f}_i(u^h), \dot{u}^h_i \right\rangle_{\Omega} \right| \leq \left( \bar{C} m + \frac{1}{2} \right) \| \dot{u}^h \|^2 + \bar{C} \tilde{f}_i(0).
\]
Using (2.21), (3.9) and (3.13) in (3.7) gives
\[
(3.14) \quad \frac{d}{dt} \| \dot{u}^h \|^2_{J} + 2 \sum_{i=1}^{m} D_i |\dot{u}^h_i|^2 \leq \left\langle J \left( 2\bar{C} m + 1 - \nabla \cdot a(\mathcal{A}(\xi), t) \right) \dot{u}^h, \dot{u}^h \right\rangle_{\Omega}\]
\[
+ 2\bar{C} \tilde{f}(0).
\]
Finally, integrating in time and applying Gronwall’s lemma we have
\[
(3.15) \quad \| \dot{u}^h(t) \|^2_{J} \leq \left( \| \dot{u}^h(0) \|^2_{J} + 2\bar{C} \tilde{f}(0) \right) \exp \left( \sup_{\Omega \times [0,T]} \left\{ 2\bar{C} m + 1 - \nabla \cdot a(\mathcal{A}(\xi), t) \right\} t \right).
\]
From (2.16), the dilution term \(\nabla \cdot a\) has the same sign as \(\partial_t J\) and is therefore positive (or negative) if the domain is growing (or contracting). Thus, domain growth has a diluting effect on the \(L_2(\Omega_t)^m\) norm (c.f., (2.20)) of the solution.

3.5. Fully discrete scheme. We divide the time interval \([0, T]\) into \(N\) subintervals, \(0 = t_0 < \ldots < t_N = T\) and denote by \(\tau_n := t_n - t_{n-1}\) the (possibly nonuniform) time step and \(\tau = \max_n \tau_n\). We consistently use the following shorthand for a function of time: \(f^n := f(t_n)\), we denote by \(\partial f^n := \tau_n^{-1} \left( f^n - f^{n-1} \right)\).

For the approximation in time we use a modified implicit Euler method where linear reaction terms and the diffusive term are treated implicitly while the nonlinear reaction terms are treated semi-implicitly using values from the previous timestep (a 1-step Picard linearisation). Our choice of timestepping scheme stems from the numerical investigation conducted by Madzvamuse \([18]\).
The fully discrete scheme we employ to approximate the solution of Problem 1.1 is thus, find \( \hat{U}_i^n \in \hat{V} \), for \( n = 1, \ldots, N \), such that for \( i = 1, \ldots, m \), we have
\[
(3.16) \quad \left\{ \begin{array}{l}
\partial_t \left[ J U_i^n \right] + D_i \left[ J^2 B \nabla U_i^n \right] = \left[ \int J^n \hat{F}_i (U_i^{n-1}) \right] \Phi, \\
U_i^0 = \Lambda^n u_i^0,
\end{array} \right. \quad \forall \Phi \in \hat{V},
\]
where \( \Lambda^n \) is the Lagrange interpolant and \( F_i \) is as defined in (2.28).

3.6. **Moving mesh formulation.** Alternatively, and in a more physically intuitive way, we may look to approximate the solution to (1.1) on a conforming subspace of the evolving domain. To this end we define a family of finite dimensional spaces \( V^n, n = 0, \ldots, N \) such that with \( \Phi \) as defined in (3.2):
\[
(3.17) \quad V^n := \left\{ \Phi^n \in H^1 (\Omega^n) : \Phi^n (\mathcal{A}_n (\xi)) = \tilde{\Phi} (\xi) \right\},
\]
which also defines the triangulation \( \mathcal{T}^n, n = 0, \ldots, N \) on the evolving domain. Using (3.16) and (3.17) we have the following equivalent finite element formulation on the evolving domain: find \( \hat{U}_i^n \in V^n \), for \( n = 1, \ldots, N \), such that for \( i = 1, \ldots, m \),
\[
(3.18) \quad \left\{ \begin{array}{l}
\partial_t \left[ (U_i, \Phi)_{\Omega_i} \right] + D_t \left[ \nabla U_i^n, \nabla \Phi^n \right]_{\Omega_i} = \left[ \int U_i^n \tilde{F}_i (U_i^{n-1}) \Phi^n \right]_{\Omega_i}, \\
U_i^0 = \Lambda^n u_i^0,
\end{array} \right. \quad \forall \Phi \in V^n,
\]
where \( \Lambda^n : H^1 (\Omega_i^n) \rightarrow V_0 \) is the Lagrange interpolant. By (2.19) and (3.17)
\[
(3.19) \quad \partial_t \tilde{\Phi} (\xi) = \left[ \partial_t \Phi + a \cdot \nabla \Phi \right] (\mathcal{A}_i (\xi)) = 0.
\]

4. **Analysis of the semidiscrete scheme**

We now prove that the semidiscrete solution converges to the exact one with optimal order in the \( L_{\infty} (0, T; L^2 (\hat{\Omega}^m)) \) norm and the \( L_2 (0, T; H^1 (\hat{\Omega}^m)) \) seminorm.

4.1. **A time-dependent Ritz projection.** A central role in the analysis is played by the Ritz, or elliptic, projector, defined, as in Wheeler [31], for each \( t \in [0, T] \), by \( R_t : H^1 (\hat{\Omega}) \rightarrow \hat{V} \) such that for each \( \hat{v} \in H^1 (\hat{\Omega}) \)
\[
(4.1) \quad b_t \left( \hat{v}, \hat{\Phi} \right) = b_t \left( R_t \hat{v}, \hat{\Phi} \right) \quad \forall \hat{\Phi} \in \hat{V},
\]
\[
(4.2) \quad \int_{\hat{\Omega}} [R_t \hat{v} - \hat{v}] = 0.
\]
The constraint (4.2) ensures \( R_t \) is well defined. Differentiation in time in (4.1) with \( v = \hat{u}_i \) yields
\[
(4.3) \quad b \left( \partial_t (\hat{u}_i - R \hat{u}_i), \hat{\Phi} \right) + \left( \partial_t \tilde{A} \nabla (\hat{u}_i - R \hat{u}_i), \nabla \hat{\Phi} \right)_{\hat{\Omega}} = 0, \quad \forall \hat{\Phi} \in \hat{V}.
\]
To obtain optimal error estimates, we now decompose the error into an **elliptic error** (the error between the Ritz projection and the exact solution) and a **parabolic error** (the error between the semidiscrete solution and the Ritz projection):
\[
(4.4) \quad \hat{u}^h - \hat{u} = (\hat{u}^h - R \hat{u}) + (R_t \hat{u} - \hat{u})
\]
4.2. Lemma (Ritz projection error estimate). Suppose assumptions \(2.6\) and \(2.3\) (with \(k = \ell\)) hold and let \(R\) be the Ritz projection defined in \((4.1)\). Then the following estimates hold:

\begin{align}
(4.5) \quad & \sup_{t \in [0,T]} \left\{ \| R_{t} \hat{u}(t) - \hat{u}(t) \|_{L^{2}(\hat{\Omega})}^{2} + \hat{h}^{2} \sum_{i=1}^{m} \| \nabla \left( R_{t} \hat{u}_{i}(t) - \hat{u}_{i}(t) \right) \|_{L^{2}(\hat{\Omega})}^{2} \right\} \leq C(\mathcal{A}, \hat{u}) \hat{h}^{2(\ell + 1)}, \\
(4.6) \quad & \sup_{t \in [0,T]} \left\{ \| \partial_{t}( R_{t} \hat{u}(t) - \hat{u}(t) ) \|_{L^{2}(\hat{\Omega})}^{2} + \hat{h}^{2} \sum_{i=1}^{m} \| \nabla \partial_{t} \left( R_{t} \hat{u}_{i}(t) - \hat{u}_{i}(t) \right) \|_{L^{2}(\hat{\Omega})}^{2} \right\} \leq C(\mathcal{A}, \hat{u}) \hat{h}^{2(\ell + 1)}. 
\end{align}

**Proof.** Using \((2.23)\) and \((4.1)\) we have for \(i = 1, \ldots, m\)

\begin{equation}
\mu \| \nabla \hat{\varepsilon}_{i} \|_{L^{2}(\hat{\Omega})}^{2} \leq a(\hat{\varepsilon}_{i}, \hat{\Phi} - \hat{u}) \quad \forall \hat{\Phi} \in \hat{V}
\end{equation}

\begin{equation}
= \hat{\mu} \| \nabla \hat{\varepsilon}_{i} \|_{L^{2}(\hat{\Omega})} \| \nabla( T^{\hat{h}} \hat{u}_{i} - \hat{u}) \|_{L^{2}(\hat{\Omega})} \leq C \hat{\mu} \| \nabla \hat{\varepsilon}_{i} \|_{L^{2}(\hat{\Omega})} \| \hat{u}_{i} \|_{H^{\ell+1}(\hat{\Omega})},
\end{equation}

which shows the energy norm bound of \((4.5)\). To show the \(L^{2}\) estimate we use duality. Fix a \(t \in (0,T]\) and consider the solution \(\hat{\psi}\) of following elliptic problem

\begin{equation}
- \nabla \cdot ( B_{i} \nabla \hat{\psi} ) = \hat{\phi} \text{ in } \hat{\Omega}, \quad B_{i} \nabla \hat{\psi} \cdot \hat{\nu} = 0 \text{ on } \partial \hat{\Omega}, \quad \int_{\hat{\Omega}} \hat{\psi} = 0.
\end{equation}

Note that \(\| \hat{\psi} \|_{L^{2}(\hat{\Omega})} \leq C \| \hat{\phi} \|_{H^{1}(\hat{\Omega})}\) as for any \(\hat{\psi}\)

\begin{equation}
\inf_{r \in R} \| \hat{\psi} - r \|_{L^{2}(\hat{\Omega})} = \left\| \hat{\psi} - \frac{1}{|\hat{\Omega}|} \int_{\hat{\Omega}} \hat{\phi} \right\|_{L^{2}(\hat{\Omega})} \leq C \| \hat{\phi} \|_{H^{1}(\hat{\Omega})}.
\end{equation}

We therefore have

\begin{equation}
\mu \| \nabla \hat{\psi} \|_{L^{2}(\hat{\Omega})}^{2} \leq b_{i} \left( \hat{\psi}, \hat{\psi} \right)_{\hat{\Omega}} \leq C \| \nabla \hat{\psi} \|_{L^{2}(\hat{\Omega})}.
\end{equation}

Furthermore we have the estimate

\begin{equation}
\| \hat{\psi} \|_{H^{2}(\hat{\Omega})} \leq C \| \Delta \hat{\phi} \|_{L^{2}(\hat{\Omega})} \leq C \| B \Delta \hat{\psi} \|_{L^{2}(\hat{\Omega})} = C \| \hat{\phi} + \nabla \cdot B \cdot \nabla \hat{\psi} \|_{L^{2}(\hat{\Omega})} \leq C \| \hat{\phi} \|_{L^{2}(\hat{\Omega})}.
\end{equation}

Here we have introduced the notation that the divergence of the tensor \(B\) is a vector defined such that for \(i = 1, \ldots, d\)

\begin{equation}
\langle \nabla \cdot B \rangle_{i} = \sum_{j=1}^{d} \partial_{x_{j}} B_{i,j}.
\end{equation}

Thus testing \((4.8)\) with \(\hat{\varepsilon}_{i}\) and using \((4.1)\) we have

\begin{equation}
\left\langle \hat{\varepsilon}_{i}, \hat{\phi} \right\rangle_{\hat{\Omega}} = b_{i} \left( \hat{\varepsilon}_{i}, \hat{\psi} - \hat{\Phi} \right) \quad \forall \hat{\Phi} \in \hat{V}
\end{equation}

\begin{equation}
\leq \mu \| \nabla \hat{\varepsilon}_{i} \|_{L^{2}(\hat{\Omega})} \| \nabla( T^{\hat{h}} \hat{\psi} ) \|_{L^{2}(\hat{\Omega})} \leq C \hat{\mu} \| \hat{\varepsilon}_{i} \|_{H^{\ell+1}(\hat{\Omega})} \| \hat{\psi} \|_{H^{2}(\hat{\Omega})} \leq C \hat{\mu} h^{\ell+1},
\end{equation}

which completes the proof of \((4.5)\). For the proof of \((4.6)\) we have using \((4.3)\) and the fact that the gradient commutes with the time derivative (as we work on the reference domain) that for \(i = 1, \ldots, m\), and for each \(\hat{\Phi} \in \hat{V},

\begin{equation}
\mu \| \nabla \partial_{t} \hat{\varepsilon}_{i} \|_{L^{2}(\hat{\Omega})}^{2} \leq b_{i} \left( \partial_{t} \hat{\varepsilon}_{i}, \hat{\Phi} - \partial_{t} \hat{u}_{i} \right) + b_{i} \left( \partial_{t} \hat{\varepsilon}_{i}, \partial_{t} R_{t} \hat{u}_{i} - \hat{\Phi} \right)
\end{equation}

\begin{equation}
= b_{i} \left( \partial_{t} \hat{\varepsilon}_{i}, \hat{\Phi} - \partial_{t} \hat{u}_{i} \right) + \left\langle \partial_{t} B \nabla \hat{\varepsilon}_{i}, \nabla( \hat{\Phi} - \partial_{t} R_{t} \hat{u}_{i} ) \right\rangle_{\hat{\Omega}}.
\end{equation}
Taking $\Phi = I_h \partial_t u_\ell$ in (4.14) gives
\[
\mu \| \nabla \partial_t \xi_i \|^2_{L^2(\Omega)} \leq C \hat{h}^2 \| \partial_t u_\ell \|_{H^{\ell+1}(\Omega)} \| \nabla \partial_t \xi_i \|_{L^2(\Omega)}
\]
(4.15)
\[
+ \|B \|_{L^\infty(\hat{\Omega})} \| \nabla \xi_i \|_{L^2(\hat{\Omega})} \left( \| \nabla \partial_t \xi_i \|_{L^2(\hat{\Omega})} + \| \nabla \left( \left. T^h \partial_t u_\ell \right|_{\hat{\Omega}} - \partial_t u_\ell \right) \|_{L^2(\hat{\Omega})} \right)
\]
\[
\leq \frac{\mu}{2} \| \nabla \partial_t \xi_i \|^2_{L^2(\hat{\Omega})} + C \| \nabla \xi_i \|^2_{L^2(\hat{\Omega})} + \hat{h}^{2\ell} \| \partial_t u_\ell \|^2_{H^{\ell+1}(\Omega)},
\]
where we have used Young’s inequality in the final step. The previous estimate (4.3) completes the proof of the energy norm bound in (4.6). For the $L^2$ estimate we once again use duality. Testing problem (4.3) with $\partial_t \xi_i$ and using (4.3), we have for $i = 1, \ldots, m$, and any $\Phi \in \tilde{V}$
\[
\left\langle \partial_t \xi_i, \phi \right\rangle_{\hat{\Omega}} = b_t \left( \partial_t \xi_i, \psi - \Phi \right) - \left\langle \left( \partial_t B \right) \nabla \xi_i, \nabla \phi \right\rangle_{\hat{\Omega}}
\]
(4.16)
\[
= b_t \left( \partial_t \xi_i, \psi - \Phi \right) + \left\langle \left( \partial_t B \right) \nabla \xi_i, \nabla \left( \psi - \Phi \right) \right\rangle_{\hat{\Omega}} - \left\langle \left( \partial_t B \right) \nabla \xi_i, \nabla \psi \right\rangle_{\hat{\Omega}}.
\]
Taking $\Phi = I_h \partial_t u_\ell$ in (4.16) gives
\[
\left\| \right. \left. \left\langle \partial_t \xi_i, \phi \right\rangle_{\hat{\Omega}} \right\| \leq C \left\| \nabla \partial_t \xi_i \right\|_{L^2(\hat{\Omega})}
\]
(4.17)
\[
+ \hat{h} \left\| \partial_t B \right\|_{L^\infty(\hat{\Omega})} \left\| \nabla \xi_i \right\|_{L^2(\hat{\Omega})} + \left\| \partial_t B \right\|_{L^\infty(\hat{\Omega})} \left\| \xi_i \right\|_{L^2(\hat{\Omega})}
\]
\[
+ \left\| \nabla \psi \right\|_{L^2(\hat{\Omega})} \left\| \partial_t B \right\|_{L^\infty(\hat{\Omega})} \left\| \xi_i \right\|_{L^2(\hat{\Omega})},
\]
where we have used integration by parts to estimate the last term in (4.16). The previous estimates and Assumption 2.3 complete the proof. □

4.3. Theorem (A priori estimate for the semidiscrete scheme). Suppose Assumptions 2.5 and 2.6 hold. Furthermore, let Assumption 2.3 hold (with $k = \ell$). Finally let $\tilde{u}^h$ be the solution to Problem 3.6. Then, the following optimal a priori error estimate holds for the error in the semidiscrete scheme:
\[
\sup_{t \in [0,T]} \left\{ \left\| \tilde{u}^h(t) - \tilde{u}(t) \right\|_{L^2(\Omega)}^2 + \sum_{i=1}^m \int_0^T \hat{h}^2 \left\| \nabla (\tilde{u}^h(t) - \tilde{u}(t)) \right\|_{L^2(\Omega)}^2 \, dt \right\} \leq C \left( A, \tilde{u}, \tilde{C} \right) \hat{h}^{2(\ell+1)},
\]
(4.18)

Proof. Using the decomposition (4.4) and Lemma 4.2 we have a bound on the elliptic error and it simply remains to estimate the parabolic error $\tilde{\rho}^h$. To this end, we use (3.6) to construct a PDE for $\tilde{\rho}^h$ by inserting $\rho^h_i$ in place of $\tilde{u}^h$ and taking $\Phi = \rho^h_i$. Using (2.21) we obtain for $i = 1, \ldots, m$,
\[
\left\langle \partial_t \left( J \rho^h_i \right), \rho^h_i \right\rangle_{\hat{\Omega}} + D_1 \left\| \nabla \rho^h_i \right\|_{\tilde{B}}^2 = \left\langle \tilde{f}_i(\tilde{u}^h), J \rho^h_i \right\rangle_{\hat{\Omega}} - \left\langle \partial_t (J R_1 \tilde{u}_i), \rho^h_i \right\rangle_{\hat{\Omega}} - b_t \left( \nabla R_1 \tilde{u}_i, \nabla \rho^h_i \right).
\]
(4.19)

Using (2.30), (2.32) and (4.1) gives
\[
\left\langle \partial_t \left( J \rho^h_i \right), \rho^h_i \right\rangle_{\hat{\Omega}} + D_1 \left\| \nabla \rho^h_i \right\|_{\tilde{B}}^2 = \left\langle \tilde{f}_i(\tilde{u}^h) - \tilde{f}_i(\tilde{u}), J \rho^h_i \right\rangle_{\hat{\Omega}} - \left\langle \partial_t (J \xi_i), \rho^h_i \right\rangle_{\hat{\Omega}}.
\]
(4.20)

Dealing with the first term on the left of (4.20) as in (3.9):
\[
\left\langle \partial_t \left( J \rho^h_i \right), \rho^h_i \right\rangle_{\hat{\Omega}} = \frac{1}{2} \left\| \frac{d}{dt} \rho^h_i \right\|_{\tilde{B}}^2 + \left\langle J \rho^h_i \nabla \cdot a(A_\ell(\xi)), \rho^h_i \right\rangle_{\hat{\Omega}}.
\]
(4.21)
Dealing with the first term on the right of (4.20) using (4.4) and the MVT we have

\[ (4.22) \quad \left| \left\langle \tilde{f}_i(u^h) - \tilde{f}_i(u), J\hat{\rho}_i^h \right\rangle_{\Omega} \right| \leq \tilde{C} \left( \sum_{j=1}^{m} \left( |\hat{\varepsilon}_j| + |\hat{\rho}_j^h| \right), J|\hat{\rho}_i^h| \right)_{\Omega}. \]

Applying Young’s inequality:

\[ (4.23) \quad \left| \left\langle \tilde{f}_i(u^h) - \tilde{f}_i(u), J\hat{\rho}_i^h \right\rangle_{\Omega} \right| \leq \tilde{C} \left( \frac{3m}{2} \|\hat{\rho}_i^h\|_J^2 + \frac{m}{2} \|\hat{\varepsilon}_i\|_{J^m}^2 \right). \]

Summing over \(i\) we have

\[ (4.24) \quad \sum_{i=1}^{m} \left| \left\langle \tilde{f}_i(u^h) - \tilde{f}_i(u), J\hat{\rho}_i^h \right\rangle_{\Omega} \right| \leq \tilde{C} \left( \frac{3m}{2} \|\hat{\rho}_i^h\|_J^2 + \frac{m}{2} \|\hat{\varepsilon}_i\|_{J^m}^2 \right). \]

Dealing with the first term on the right of (4.20):

\[ (4.25) \quad \left| \left\langle \partial_t (J\hat{\varepsilon}_i), \hat{\rho}_i^h \right\rangle_{\Omega} \right| \leq \left| \left\langle J\partial_t \hat{\varepsilon}_i, \hat{\rho}_i^h \right\rangle_{\Omega} \right| + \left| \left\langle \partial_t (J) \hat{\varepsilon}_i, \hat{\rho}_i^h \right\rangle_{\Omega} \right| \]

\[ \leq \frac{1}{2} \left( \|\hat{\rho}_i^h\|_J^2 + \|J\partial_t \hat{\varepsilon}_i, \hat{\rho}_i^h\|_{\Omega} + \|\partial_t (J) \hat{\varepsilon}_i, \hat{\rho}_i^h\|_{\Omega} + \{\partial_t (J) \hat{\varepsilon}_i, \hat{\rho}_i^h\}_{\Omega} \right), \]

where we have used Young’s inequality for the second step. Now using (2.16) and summing over \(i\) we have

\[ (4.26) \quad \sum_{i=1}^{m} \left| \left\langle \partial_t (J\hat{\varepsilon}_i), \hat{\rho}_i^h \right\rangle_{\Omega} \right| \leq \frac{1}{2} \left( \|\hat{\rho}_i^h\|_{J^m}^2 + \left\langle J\hat{\rho}_i^h, \nabla \cdot \mathcal{A}(\xi, t) \right\rangle_{\Omega^m} + \|\partial_t \hat{\varepsilon}_i\|_{J^m}^2 + 2 \|\partial_t J\|_{L_\infty(\tilde{\Omega} \times [0, T])} \|\hat{\varepsilon}_i\|_{L_2(\tilde{\Omega})}^2 \right). \]

Combining (4.24), (4.26)

\[ (4.27) \quad \frac{d}{dt} \|\hat{\rho}_i^h\|_{J^m}^2 + 2 \sum_{i=1}^{m} D_i |\nabla \hat{\rho}_i^h|_{\tilde{\Omega}}^2 \leq \tilde{C} \left( \|\hat{\rho}_i^h\|_{J^m}^2 + \|\hat{\varepsilon}_i\|_{L_2(\tilde{\Omega})}^2 + \|\partial_t \hat{\varepsilon}_i\|_{L_2(\tilde{\Omega})}^2 \right), \]

where we have used the fact that Assumption 2.3 implies \(J, \partial_t J \in L_\infty (\tilde{\Omega} \times [0, T])\). Integrating in time, using Lemma 4.2 and applying Gronwall’s Lemma we have

\[ (4.28) \quad \|\hat{\rho}_i^h(t)\|_{J^m}^2 + 2 \sum_{i=1}^{m} D_i \int_0^T |\nabla \hat{\rho}_i^h|_{\tilde{\Omega}}^2 \leq \tilde{C} \left( \|\hat{\rho}_i^h(0)\|_{J^m}^2 + \tilde{K}^{2(\ell+1)} \right). \]

To estimate \(\hat{\rho}_i^h(0)\), we note

\[ (4.29) \quad \|\hat{\rho}_i^h(0)\|_{J^m}^2 \leq \|\hat{u}(0) - \hat{\rho} h(0)\|_{J^m} + \|\hat{\varepsilon}_i\|_{J^m} \leq \tilde{C} h^{\ell+1}, \]

where we have used (3.3), the assumption on the regularity of the exact solution and Lemma 4.2 in the last step. Assumption 2.3 and the equivalence of norms (2.20) completes the proof. \(\square\)

5. Error analysis of the fully discrete approximation

In this section we provide the convergence result for the fully discrete scheme (3.16). The main result of this paper is Theorem 5.1, whose proof will give in details. We follow that up with a convergence result in the \(L_\infty(\tilde{\Omega})\) norm which allows the use of the original \(f\) (without extending to \(f\) in the numerical method).
5.1. Theorem (A priori estimate for the fully discrete scheme). Suppose Assumptions 2.5 and 2.6 hold. Furthermore, suppose Assumption 2.3 (with \(k = \ell\)) holds. Let \(\hat{U}\) be the solution to (3.16). Finally, suppose the timestep satisfies a stability condition defined in (5.11). Then, the following optimal a priori estimate holds for the error in the fully discrete scheme:

\[
\|\hat{U}^n - \hat{u}^n\|_{L_2(\hat{\Omega})}^2 + h^2 \sum_{i=1}^{m} D_i \|\nabla \left(\hat{U}_i^n - \hat{u}_i^n\right)\|_{L_2(\hat{\Omega})}^2 \\
\leq C\left(\mathcal{A}, \hat{u}, \mathcal{C}\right) \left(h^{2(\ell+1)} + \tau^2\right), \quad \text{for } n \in \{0, \ldots, N\},
\]

(5.1)

5.2. Remark (Error estimate for the evolving domain scheme). The schemes (3.16) and (3.18) are equivalent up-to numerical quadrature. Thus Theorem 5.1 also provides an error estimate for the evolving domain based scheme (3.18).

Proof of Theorem 5.1. Decomposing the error as in (4.4) we have

\[
\|\hat{U}^n - \hat{u}^n\|_{L_2(\hat{\Omega})}^2 \leq \|R_i \hat{u}_i^n - \hat{u}_i^n\|_{L_2(\hat{\Omega})}^2 + \|\hat{U}^n - R_i \hat{u}_i^n\|_{L_2(\hat{\Omega})}^2 = \|\hat{e}^n\|_{L_2(\hat{\Omega})}^2 + \|\hat{\rho}^n\|_{L_2(\hat{\Omega})}^2.
\]

(5.2)

From Lemma 4.2 we have the following bound on the elliptic error:

\[
\|\hat{e}^n\|_{L_2(\hat{\Omega})}^2 \leq C h^{2(\ell+1)} \quad \text{for } n \in \{0, \ldots, N\}.
\]

(5.3)

Therefore it only remains to estimate \(\hat{\rho}^n\). Constructing an expression for \(\hat{\rho}^n\) as in (4.19), using (3.16) and (4.1) we obtain for \(i = 1, \ldots, m,\)

\[
\langle \hat{\partial} [J \hat{\rho}]^n, \hat{\rho}^n \rangle_{\hat{\Omega}} = \frac{1}{\tau_n} \left(\|\hat{\rho}^n\|_{\Omega}^2 - \frac{1}{2} \langle [J^{n-1} \hat{\rho}_i^n, \hat{\rho}_i^n]_{\Omega} + \langle [J^{n-1} \hat{\rho}_i^n, \hat{\rho}_i^n]_{\Omega} \right)\right)
\]

(5.4)

where we have used (2.30) for the second step and \(\hat{\Phi}\) is as defined in (2.31). Using Young’s inequality for the first term on the left hand side of (5.4) gives

\[
\langle \hat{\partial} [J \hat{\rho}]^n, \hat{\rho}^n \rangle_{\hat{\Omega}} \geq \frac{1}{\tau_n} \left(\|\hat{\rho}^n\|_{\Omega}^2 - \frac{1}{2} \langle [J^{n-1} \hat{\rho}_i^n, \hat{\rho}_i^n]_{\Omega} + [J^{n-1} \hat{\rho}_i^n, \hat{\rho}_i^n]_{\Omega} \right)\right)
\]

(5.5)

where we have used (2.20). Summing over \(i\) we have

\[
\sum_{i=1}^{m} \langle \hat{\partial} [J \hat{\rho}]^n, \hat{\rho}^n \rangle_{\hat{\Omega}} \geq \frac{1}{\tau_n} \left(1 - \frac{1}{2} \|\hat{\rho}^n\|_{\Omega}^2 \|J^{n-1}\|_{L_{\infty}(\hat{\Omega})} \right) \|\hat{\rho}^n\|_{J^m}^2 - \frac{1}{2\tau_n} \|\hat{\rho}^n\|_{J^m}^2.
\]

(5.6)
Using (5.2) and the MVT for the first term on the right of (5.4) gives
\[
\left\langle \tilde{U}_i^n \tilde{F}_i \left( \tilde{U}^{n-1} \right) - \tilde{f}_i(\tilde{u}^n), [J\hat{\rho}_i]^n \right\rangle \Omega
\]
\[
\leq \tilde{C} \sum_{j=1}^m \left( \|\hat{\rho}_j^n\|^2 J_J^n + \|\tau_n \partial \hat{u}_j^n\| + \|\tilde{\varepsilon}_j^n\| + \|\hat{\rho}_j^n\| + \|J^n\|_{L_\infty}(\Omega) \|\hat{\rho}^{n-1}\|_{J_J^n} \right) \Omega
\]
(5.7)
\[
\leq C \tilde{C} \left( \|\hat{\rho}_i^n\|^2 J_J^n + \|\tau_n \partial \hat{u}_i^n\| + \|\tilde{\varepsilon}_i^n\| + \|\hat{\rho}_i^n\| + \|J^n\|_{L_\infty}(\Omega) \|\hat{\rho}^{n-1}\|_{J_J^n} \right)
\]
where we have used Young’s inequality for the second step. Summing over \(i\) we have
\[
\sum_{i=1}^m \left\langle \tilde{U}_i^n \tilde{F}_i \left( \tilde{U}^{n-1} \right) - \tilde{f}_i(\tilde{u}^n), [J\hat{\rho}_i]^n \right\rangle \Omega
\]
(5.8)
\[
\leq C \tilde{C} \left( \|\hat{\rho}^n\|_{J_J^n}^2 + \|\tau_n \partial \hat{u}^n\| + \|\tilde{\varepsilon}^n\| + \|\hat{\rho}^{n-1}\|_{J_J^n} \right)
\]
Applying Young’s inequality to the second and third term on the right of (5.4) gives
\[
\left\langle \partial [J\tilde{\varepsilon}_i^n], \hat{\rho}_i^n \right\rangle_{\Omega} + \left\langle \left( \partial - \partial_t \right) [J\hat{u}_i^n], \hat{\rho}_i^n \right\rangle_{\Omega}
\]
\[
\leq \|\hat{\rho}_i^n\|_{J_J^n}^2 + \frac{1}{2} \|\partial [J\tilde{\varepsilon}_i^n]\|_{L_2(\hat{\Omega})}^2 + \|\partial - \partial_t\|_{L_2(\hat{\Omega})}^2
\]
(5.9)
Using (5.6), (5.8) and (5.9) in (5.4) gives
\[
\frac{1}{\tau_n} \left( 1 - \frac{1}{2} \|J^n\|_{L_\infty}(\hat{\Omega}) \right) - C \tilde{C} \tau_n \|\hat{\rho}^n\|_{L_2(\hat{\Omega})}^2 + \sum_{i=1}^m \|D_i^\tau \|\nabla \hat{\rho}_i^n\|_{L_2(\hat{\Omega})}^2
\]
(5.10)
\[
\leq \left( \frac{1}{2\tau_n} + C \tilde{C} \|J^n\|_{L_\infty}(\hat{\Omega}) \right) \|\hat{\rho}^{n-1}\|_{J_J^n}^2 + C \tilde{C} \|J^n\|_{L_\infty}(\hat{\Omega}) \left( \|\tilde{\varepsilon}^n\|^2_{L_2(\hat{\Omega})} + \|\tilde{\varepsilon}^{n-1}\|^2_{L_2(\hat{\Omega})} + \|\tau_n \partial \hat{u}^n\|_{L_2(\hat{\Omega})}^2 \right)
\]
\[
+ \frac{1}{2} \|\partial [J\tilde{\varepsilon}^n]\|_{L_2(\hat{\Omega})}^2 + \|\partial - \partial_t\|_{L_2(\hat{\Omega})}^2
\]
Let \(\tau' > 0\) be such that, for \(\tau < \tau'\) and for \(n = 1, \ldots, N\),
\[
1 - \frac{1}{2} \|J^n\|_{L_\infty}(\hat{\Omega}) - C \tilde{C} \tau > 0.
\]
(5.11)
Such a \(\tau'\) exists since
\[
\lim_{\tau \to 0} \left\{ \frac{1}{2} \|J^n\|_{L_\infty}(\hat{\Omega}) + C \tilde{C} \tau \right\} = \frac{1}{2}.
\]
(5.12)
For \( \tau < \tau' \), we have

\[
\|
\dot{\rho}^n \|^2_{L^2} + \sum_{i=1}^{m} C \tau D_i \left| \nabla \hat{\rho}_i^n \right|_{L^2} \leq C \left( \tilde{C} \|
\dot{\rho}^{n-1} \|^2_{L^2} + \tau R^n \right),
\]

where \( \tilde{C} = 1 + \tau \tilde{C} \| \frac{J^n}{J} \|_{L^\infty(\hat{\Omega})} \) and

\[
R^n := \tilde{C} \left| J^n \right|_{L^\infty(\hat{\Omega})} \left( \| \hat{\epsilon}^n \|^2_{L^2(\hat{\Omega})^m} + \| \hat{\epsilon}^{n-1} \|^2_{L^2(\hat{\Omega})^m} + \| \tau \hat{\partial} \hat{u}^n \|^2_{L^2(\hat{\Omega})^m} \right)
+ \frac{1}{2} \left| J^n \right|_{L^\infty(\hat{\Omega})} \left( \| \hat{\partial} \hat{J} \hat{e}^n \|^2_{L^2(\hat{\Omega})^m} + \| \hat{\partial} (\hat{\partial} \hat{u}) \|^2_{L^2(\hat{\Omega})^m} \right).
\]

Therefore, for \( n = 1, \ldots, N \),

\[
\|
\dot{\rho}^n \|^2_{L^2} + \sum_{i=1}^{m} C \tau D_i \left| \nabla \hat{\rho}_i^n \right|_{L^2} \leq C \left( \prod_{k=1}^{n} \tilde{C} \| \dot{\rho}^n \|^2_{L^2} + \tau \sum_{j=1}^{n} \prod_{k=1}^{j} C \tilde{C} R^j \right).
\]

Considering the first two terms on the right of (5.14), we have for \( n = 1, \ldots, N \)

\[
\tilde{C} \left| J^n \right|_{L^\infty(\hat{\Omega})} \left( \| \hat{\epsilon}^n \|^2_{L^2(\hat{\Omega})^m} + \| \hat{\epsilon}^{n-1} \|^2_{L^2(\hat{\Omega})^m} \right)
\leq 2 \tilde{C} \sup_{s \in [0, \ldots, N]} \left| J^s \right|_{L^\infty(\hat{\Omega})} \| \hat{\epsilon}^s \|^2_{L^2(\hat{\Omega})^m}
\leq \tilde{C} \hat{C} t^{2(\ell+1)},
\]

where we have used Assumption 2.3 and Lemma 4.2. Dealing with the third term on the right of (5.14), we have

\[
\tilde{C} \left| J^n \right|_{L^\infty(\hat{\Omega})} \| \tau \hat{\partial} \hat{u}^n \|^2_{L^2(\hat{\Omega})^m} = \tilde{C} \left| J^n \right|_{L^\infty(\hat{\Omega})} \left| \int_{t_{n-1}}^{t_n} \hat{\partial} \hat{u}^s \, ds \right|^2_{L^2(\hat{\Omega})^m}
\leq \tilde{C} \hat{C} \tau^2,
\]

where we have used Assumptions 2.4 and 2.3. For the fourth term on the right of (5.14), we have

\[
\frac{1}{2} \left| J^n \right|_{L^\infty(\hat{\Omega})} \left| \hat{\partial} \hat{J} \hat{e}^n \right|^2_{L^2(\hat{\Omega})^m} \leq \frac{1}{2} \left| J^n \right|_{L^\infty(\hat{\Omega})} \left| \int_{t_{n-1}}^{t_n} \hat{\partial} [\hat{J} \hat{e}^s] \, ds \right|^2_{L^2(\hat{\Omega})^m}
\leq C \sup_{s \in [t_{n-1}, t_n]} \| \hat{\epsilon}^s \|^2_{L^2(\hat{\Omega})^m}
\leq C \hat{C} t^{2(\ell+1)},
\]

where we have used Assumption 2.3 for the second step and Lemma 4.2 for the final step. Finally, for the fifth term on the right of (5.14), we have

\[
\left| \frac{1}{J^n} \right|_{L^\infty(\hat{\Omega})} \left| \hat{\partial} \hat{J} \hat{u}^n \right|^2_{L^2(\hat{\Omega})^m} = \left| \frac{1}{J^n} \right|_{L^\infty(\hat{\Omega})} \left| \int_{t_{n-1}}^{t_n} \left( s - t_{n-1} \right) \hat{\partial} [\hat{J} \hat{u}^s] \, ds \right|^2_{L^2(\hat{\Omega})^m}
\leq C \tau^2 \sup_{s \in [t_{n-1}, t_n]} \left( \left| \hat{\partial} \hat{u}^s \right|^2_{L^2(\hat{\Omega})^m} + \| \hat{u}^s \|^2_{L^2(\hat{\Omega})^m} \right)
\leq C \tau^2,
\]
where we have used Assumption 2.3 for the second step and Assumption 2.6 for the final step. Combining (5.16), (5.17), (5.18) and (5.19) we have

\[ R_n \leq C \left( \hat{h}^{2(\ell+1)} + \tau^2 \right) \quad \text{for } n = 1, \ldots, N. \]

Using (4.29) we have

\[ \| \hat{\rho}_n^0 \|_{L^2} \leq \| \hat{\rho}_h^0(0) \|_{L^2} \leq C \hat{h}^{2(\ell+1)}. \]

Applying estimates (5.20) and (5.21) in (5.13) completes the proof of Theorem 5.1. □

5.3. Remark (Stability of the fully discrete scheme). The timestep restriction (5.11) is composed of a term arising from domain growth (the term involving the determinant of the diffeomorphism \( A \)) and a term arising from the nonlinear reaction kinetics (the term containing \( \tilde{C} \)). It is worth noting that for a given set of reaction kinetics, i.e., a given \( \tilde{C} \), larger timesteps are admissible on growing domains (as we have \( \| J_{n-1}/J_n \|_{L^\infty} < 1 \)). If we consider for illustrative purposes the heat equation, i.e, the case \( \tilde{C} = 0 \), we recover unconditional stability on growing domains whereas for contracting domains (5.11) implies a stability condition on the timestep dependent on the growth rate.

5.4. Remark (Qualitative estimates on the exact solution). In practice only qualitative a priori estimates are generally available for the exact solution and the region \( I_\delta \) defined in Assumption 2.6 is not explicitly known. Thus, we cannot construct the function \( \tilde{f} \) defined in (2.31). To this end, we introduce the following assumption to circumvent the construction of \( \tilde{f} \).

5.5. Assumption (Dimension dependent polynomial degree). We wish to invoke estimate (3.4) with a positive power of \( \hat{h} \) and thus we require the degree of the finite element space to satisfy

\[ \ell > \frac{d}{2} - 1, \]

where \( d \) is the spatial dimension. Thus, we require piecewise linear or higher basis functions for \( d \leq 2 \) and at least piecewise quadratics for \( d = 3 \).

5.6. Remark (Maximum-norm bound of the discrete solution). Let assumptions in 5.5 and Theorem 5.1 be valid. Then we have

\[ \| \hat{u}^n - \hat{U}^n \|_{L^\infty(\hat{\Omega})} \leq C \hat{h}^{\ell+1/2}, \]

and for sufficiently small mesh-size \( \hat{h} \) the discrete solution \( \hat{U}^n \) to Problem 3.16 is in the region \( I_\delta \) for all \( n \in [0, \ldots, N] \). Thus, we may replace \( \tilde{F} \) in (3.16) by \( F \).

Indeed, for \( n \in [0, \ldots, N] \) we have for \( \hat{T}^h \) the Clement interpolant

\[ \| \hat{u}^n - \hat{U}^n \|_{L^\infty(\hat{\Omega})} \leq \| \hat{T}^h \hat{u}^n - \hat{U}^n \|_{L^\infty(\hat{\Omega})} + \| \hat{u}^n - \hat{T}^h \hat{u}^n \|_{L^\infty(\hat{\Omega})}. \]

Using (3.4) and (5.5) gives

\[ \| \hat{u}^n - \hat{U}^n \|_{L^\infty(\hat{\Omega})} \leq C \left( \hat{h}^{-d/2} \left( \| \hat{T}^h \hat{u}^n - \hat{u}^n \|_{L^2(\hat{\Omega})} + \| \hat{u}^n - \hat{U}^n \|_{L^2(\hat{\Omega})} \right) \right)^{1/2} \]

\[ + \hat{h}^{\ell+1-d/2} \| \hat{u}^n \|_{H^{\ell+1}(\hat{\Omega})}. \]

Error bound (5.23) now follows from (3.3) and Theorem 5.1. Thus, if \( \hat{h} \) is taken sufficiently small we have

\[ \sup_{n \in [0, \ldots, N]} \| \hat{u}^n - \hat{U}^n \|_{L^\infty(\hat{\Omega})} \leq \frac{\delta}{2}. \]
Therefore, \( \hat{U}^n \in I_4 \) for all \( n \in \{0, \ldots, N\} \) and thus, \( \tilde{f}(\hat{U}) = f(\hat{U}) \).

6. IMPLEMENTATION

In this section we illustrate the implementation of the finite element scheme with explicit nonlinear reaction functions. We demonstrate that scheme (3.16) on the reference domain or scheme (3.18) on the evolving domain give rise to equivalent linear systems. To illustrate a concrete application of the proposed scheme we consider the following widely studied set of reaction kinetics.

6.1. Definition (Schnakenberg’s “activator-depleted substrate” model \([10, 15, 25]\)). We consider the following activator depleted substrate model, also known as the Brusselator model in nondimensional form:

\[
\begin{align*}
    f_1(u_1, u_2) &= \gamma (a - u_1 + u_1^2 u_2), \\
    f_2(u_1, u_2) &= \gamma (b - u_1^2 u_2),
\end{align*}
\]

where \( 0 < a, b, \gamma < \infty \).

In matrix vector form scheme (3.16) equipped with kinetics (6.1) and appropriate initial approximations \( W^n_0, W^n_2 \): is: To solve for \( \hat{W}^n_1, \hat{W}^n_2 \), \( n = \{1, \ldots, N\} \), the linear systems given by

\[
\begin{align*}
    \left( \frac{1}{\tau_n} \hat{M}^n + D_1 \hat{S}^n + \gamma \hat{N}_1 \right) \hat{W}^n_1 &= \frac{1}{\tau_n} \hat{M}^{n-1} \hat{W}^{n-1}_1 + \gamma a \hat{F}^n, \\
    \left( \frac{1}{\tau_n} \hat{M}^n + D_2 \hat{S}^n + \gamma \hat{N}_2 \right) \hat{W}^n_2 &= \frac{1}{\tau_n} \hat{M}^{n-1} \hat{W}^{n-1}_2 + \gamma b \hat{F}^n,
\end{align*}
\]

where \( \hat{W}^n_1 \) and \( \hat{W}^n_2 \) represent the nodal values of the discrete solutions corresponding to \( \hat{u}_1 \) and \( \hat{u}_2 \) respectively and the equations are nondimensional such that either \( D_1 \) or \( D_2 \) is equal to 1. The components of the weighted mass matrix \( \hat{M} \), the weighted stiffness matrix \( \hat{S} \) and the load vector \( \hat{F} \) on the reference frame are given by

\[
\begin{align*}
    \hat{M}^{n}_{\alpha \beta} &= \int_{\Omega} J^n \hat{\Phi}_\alpha \hat{\Phi}_\beta, \\
    \hat{S}^{n}_{\alpha \beta} &= \int_{\Omega} [J K]^n \nabla \hat{\Phi}_\alpha \cdot \nabla \hat{\Phi}_\beta, \\
    \hat{F}^{n}_\alpha &= \int_{\Omega} J^n \hat{\Phi}_\alpha.
\end{align*}
\]

For reaction kinetics (6.1), the components of the matrices arising from the Picard linearisation \( \hat{N}_1 \) and \( \hat{N}_2 \) are given by

\[
\begin{align*}
    \left( \hat{N}_1 \right)_{\alpha \beta}^{\gamma} &= \sum_{\eta=1}^{\dim(\hat{Y})} \sum_{\delta=1}^{\dim(\hat{Y})} \left( [W_1^2]_{\eta \delta} \right)^{n-1} \int_{\Omega} J^n \hat{\Phi}_\alpha \hat{\Phi}_\beta \hat{\Phi}_\eta \hat{\Phi}_\delta, \\
    \left( \hat{N}_2 \right)_{\alpha \beta}^{\gamma} &= \int_{\Omega} J^n \hat{\Phi}_\alpha \hat{\Phi}_\beta + \sum_{\eta=1}^{\dim(\hat{Y})} \sum_{\delta=1}^{\dim(\hat{Y})} \left( [W_1^2]_{\eta \delta} \right)^{n-1} \int_{\Omega} J^n \hat{\Phi}_\alpha \hat{\Phi}_\beta \hat{\Phi}_\eta \hat{\Phi}_\delta,
\end{align*}
\]

respectively.

We now illustrate the implementation of scheme (3.18) where the linear systems are assembled on the evolving domain. By the definition of \( \hat{Y} \) (3.17) we obtain the following time dependent mass \( (M^n) \) and
stiffness \((S^n)\) matrices if we assemble the linear systems on the evolving domain

\[
M^n_{\alpha\beta} := \int_{\Omega_n} \Phi_n^\alpha \Phi_n^\beta = \hat{M}^n_{\alpha\beta},
\]

\[
S^n_{\alpha\beta} := \int_{\Omega_n} \nabla \Phi_n^\alpha \cdot \nabla \Phi_n^\beta = \hat{S}^n_{\alpha\beta},
\]

and the load vector on the evolving domain is given by

\[
F^n_\alpha := \int_{\Omega_n} \Phi_n^\alpha = \hat{F}^n_\alpha.
\]

We thus obtain the following linear systems:

\[
\begin{aligned}
\left( \frac{1}{\tau_n} M^n + D_1 S^n + \gamma N^n_1 \right) W^n_1 &= \frac{1}{\tau_n} M^{n-1} W^{n-1} + \gamma a F^n, \\
\left( \frac{1}{\tau_n} M^n + D_2 S^n + \gamma N^n_2 \right) W^n_2 &= \frac{1}{\tau_n} M^{n-1} W^{n-1} + \gamma b F^n,
\end{aligned}
\]

where for reaction kinetics \((6.1)\) the components of the matrices arising from the Picard linearisation \(N_1 = \hat{N}_1\) are given by

\[
(N_1)_{\alpha\beta} := \sum_{\eta=1}^{\dim(\hat{V})} \sum_{\vartheta=1}^{\dim(\hat{V})} \left[ (W_2)_{\eta\vartheta} (W_2)_{\eta\vartheta} \right]^{n-1} \int_{\Omega_n} \Phi_n^\alpha \Phi_n^\beta \Phi_n^\eta \Phi_n^\vartheta
\]

with analogous modifications for \(N_2\).

Both formulations \((6.2)\) and \((3.18)\) result in the same linear algebra problem. Solve for vectors \(b_n^i, i = 1, \ldots, m,\)

\[
A_n b_n^i = c_n^i - 1, \quad n = 1, \ldots, N.
\]

The matrix \(A^n\) is symmetric sparse and positive definite. We therefore use the conjugate gradient (CG) algorithm \([12]\) to compute the solution to the linear systems.

\[\text{Figure 1. A simple example of the reference and evolving domain with the associated mapping, mesh-size and triangulations.}\]
6.2. Remark (Quadrature on the evolving domain). As we do not have to compute the Jacobian of the mapping, assemblage of the linear systems is faster on the evolving domain. However, in the previous analysis we have neglected errors due to variational crimes, such as the fact that integrals of finite element functions must be evaluated by some numerical quadrature. In light of this, it should be noted that the finite dimensional space $V_t$ on the evolving domain will not in general consist of piecewise polynomial functions. Furthermore, simplexes on the evolving domain will not in general be affine transformations of the reference simplex (see Figure 1 for an example). If formulation (3.18) is used and domain evolution is not spatially linear, the influence of numerical quadrature on the accuracy of the scheme should be considered. We leave this extension for future studies.

7. NUMERICAL EXPERIMENTS

We now provide numerical evidence to back-up the estimate of Theorem 5.1. We use as a test problem, the Schnakenberg kinetics, although any other reaction kinetics that fulfils our assumptions could have been used. For the implementation we make use of the toolbox ALBERTA [23]. The graphics were generated with PARAVIEW [11].

7.1. Remark (Existence of solutions to Problem 1.1 with spatially linear isotropic evolution). In [30], we showed that Problem 1.1 equipped with the Schnakenberg reaction kinetics and $\Omega_t \in C^2(\Omega_t)$ is well posed under any bounded spatially linear isotropic evolution of the domain. If we assume this result holds on polygonal domains, we have sufficient regularity on the continuous problem to apply Theorem 5.1 and thus conclude scheme (3.16) with $P^1$ finite elements converges with optimal order.

7.2. Definition (Experimental order of convergence). We denote the $L_\infty(0,T;L^2(\Omega))$ error in the numerical scheme on a series of uniform refinements of a triangulation $\{\hat{T}_i\}_{i=0}^N$ by $\{\epsilon_i\}_{i=0}^N$. The experimental order of convergence (EOC) is defined to be the numerical measure of rate of convergence of the scheme as $\hat{h}_n \rightarrow 0$, where $\hat{h}_n$ denotes the maximum mesh-size of $\hat{T}_n$ and is given by

$$\text{EOC}_i(e_{i,i+1},\hat{h}_{i,i+1}) = \frac{\ln(e_{i+1}/e_i)}{\ln(\hat{h}_{i+1}/\hat{h}_i)}.$$  \hspace{1cm} (7.1)

7.3. Numerical verification of the a priori convergence rate. We examine the EOC of scheme (3.16) to approximate the solution to (1.1) with $P^1$, $P^2$ and $P^3$ basis functions and with uniform timestep $\tau \approx \hat{h}^2$, $\tau \approx \hat{h}^3$ and $\tau \approx \hat{h}^4$ respectively (since the scheme is first order in time).

We consider two different forms of domain evolution that include both domain growth and contraction to illustrate the versatility of the proposed finite element scheme.

- Spatially linear periodic evolution:

$$\mathcal{A}_t(\xi) = \xi \left( 1 + \kappa \sin \left( \frac{\pi t}{T} \right) \right).$$  \hspace{1cm} (7.2)

- Spatially nonlinear periodic evolution:

$$(\mathcal{A}_t(\xi))_i = \xi_i \left( 1 + \kappa \sin \left( \frac{\pi t}{T} \right) \xi_i \right),$$  \hspace{1cm} (7.3)

for $i = 1, \ldots, d$.

In both cases we take a time interval of $[0, 1]$, the initial domain as the unit square and the parameter $\kappa = 1$. Thus in both cases the domain grows to a square of length 2 at $t = 0.5$ before contracting back to the initial domain at end time. We take the diffusion coefficients $D = (0.01, 1)^T$ and the parameter $\gamma = 1$. Problem 1.1 equipped with nonlinear reaction kinetics does not admit any closed form solutions.
In order to provide numerical verification of the convergence rate, we insert a source term such that the exact solution is,

\[
\hat{u}_1(\xi, t) = \sin(\pi t) \exp(-10|\xi|^2), \\
\hat{u}_2(\xi, t) = -\sin(\pi t) \exp(-10|\xi|^2).
\] (7.4)

Tables 1 and 2 show the EOCs for the two benchmark examples. For the first benchmark example where domain growth is linear with respect to space, we assemble the linear systems on the evolving domain corresponding to scheme (6.11). For the second benchmark example, as domain evolution is nonlinear, we assemble the linear systems on the reference frame corresponding to scheme (6.2). In both cases we observe that the error converges at the expected rate of \( \ell + 1 \) where \( \ell \) is the degree of the finite element basis functions, providing numerical evidence for the a priori estimate of Theorem 5.1.

| \( h \) | 2^{-5/2} | 2^{-3} | 2^{-7/2} | 2^{-4} |
|---|---|---|---|---|
| \( P_1 \) | e | .119869 | .079248 | .040833 | .020521 |
| EOC | - | 1.1940 | 1.9132 | 1.9853 |
| \( P_2 \) | e | .035835 | .012380 | .004405 | .001567 |
| EOC | - | 3.0667 | 2.9816 | 2.9822 |
| \( h \) | 2^{-3/2} | 2^{-2} | 2^{-5/2} | 2^{-3} |
| \( P_3 \) | e | .153871 | .042748 | .010899 | .002728 |
| EOC | - | 3.6956 | 3.9433 | 3.9966 |

**Table 1.** Error in the \( L_\infty(0, T; L_2(\Omega)m) \) norm and EOCs for a benchmark problem with spatially linear domain evolution (7.2). The linear systems are assembled on the evolving frame corresponding to system (6.11).

| \( h \) | 2^{-5/2} | 2^{-3} | 2^{-7/2} | 2^{-4} |
|---|---|---|---|---|
| \( P_1 \) | e | .043839 | .022429 | .011133 | .005482 |
| EOC | - | 1.9337 | 2.0210 | 2.0441 |
| \( P_2 \) | e | .015906 | .005659 | .002005 | .000709 |
| EOC | - | 2.9822 | 2.9941 | 3.0010 |
| \( h \) | 2^{-3/2} | 2^{-2} | 2^{-5/2} | 2^{-3} |
| \( P_3 \) | e | .022086 | .005514 | .001375 | .000344 |
| EOC | - | 4.0038 | 4.0068 | 4.0007 |

**Table 2.** Error in the \( L_\infty(0, T; L_2(\hat{\Omega})m) \) norm and EOCs for a benchmark problem with nonlinear domain evolution (7.3). The linear systems are assembled on the reference frame corresponding to system (6.2).
7.4. **Spatial pattern formation on evolving domains.** We now present numerical results illustrating the influence of domain evolution on pattern formation by RDSs. We first present results for the Schnakenberg kinetics with domain growth functions (7.2) and (7.3) with identical initial conditions and identical numerical and reaction kinetic parameter values as given in Table 3.

We take the unit square as the initial domain and the evolution of the boundary curve of the domain is identical in both cases, with the domain growing from a square of length 1 to a square of length 5 at \( t = 1000 \) before contracting to a square of length 1 at final time. In Figures 2 and 3 we show snapshots of the discrete activator \((W_1)\) profiles obtained using the different schemes. The substrate profiles \((W_2)\) have been omitted as they are \(180^\circ\) out of phase with those of the activator. The snapshots in Figure 2 were computed using the evolving domain formulation (6.11), whilst the snapshots in Figure 3 were computed using the reference domain formulation (6.2). Considering the Figures 2 and 3, we observe that no patterns are expressed when the domain is at initial or final times. This is as expected since linear stability analysis on a fixed square with the same length as the domain at \( t = 0 \) and \( t = T \) indicates that, for the set of parameter values selected, the domain is below the critical domain size for which there exist admissible patterns. In the spatially linear case (Figure 2), an initial half spot pattern forms which continuously transitions as the domain grows into a single spot positioned in the centre of the domain. As the domain contracts this single spot disappears (via spot annihilation) with the final domain exhibiting no spatial patterning. In the spatially nonlinear growth case (Figure 3) the pattern transition is completely different with a half spot forming which splits as the domain grows to form two half spots which move around the domain before being annihilated as the domain contracts. The difference in patterning observed appears to be due to the differences in the growth function, with the results clearly illustrating the robustness of the numerical method in dealing with the complex non-uniform forms of domain evolution that are likely to be encountered in the biological problems we have in mind.

We next consider the same Schnakenberg system on a domain with evolution of the form

\[
(A_t(\xi))_i = \left(1 + 2\sin\left(\frac{\pi t}{T}\right)|\xi|^2\right)\xi_i,
\]

with final time \( T = 1000 \). We select the same parameter values as Table 3, apart from the parameter \( \gamma \) which we set equal to 1. The initial domain (and reference domain) is taken as the square \([-1, 1]^2\). Figure 4 shows the activator concentrations on a domain with evolution of the form (7.5). We observe the now familiar spot-splitting behaviour as the domain grows and spot-annihilation as the domain contracts. Interestingly, we observe that the spots appear to orient themselves to maintain a relatively uniform level of separation (which is a characteristic of Turing patterns due to their intrinsic wavelength) even with this highly nonlinear form of domain evolution.

Along with 2 component RDSs, 3 component RDSs where a second inhibitor quenches established maximums have been widely studied 20. Many interesting phenomena, which do not occur in 2 component systems, such as out of phase oscillations and space-time patterning which does not reach a steady state (even on fixed domains) are observed. The applications of such 3 component systems are of much importance, for example in the modelling of cell polarisation during chemotaxis 19. To illustrate the versatility of our method in dealing with multiple component systems, we now present results for a three

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**Table 3.** Parameter values for numerical experiments with the Schnakenberg kinetics.

| \( D_1 \) | \( D_2 \) | \( \gamma \) | \( a \) | \( b \) | \( \kappa \) | \( T \) | \( \tau \) | \( \text{DOFs} \) |
|---|---|---|---|---|---|---|---|---|
| .01 | 1.0 | 0.1 | 0.1 | 0.9 | 4 | 2000 | \( 10^{-2} \) | 8321 |
Figure 2. Snapshots of the discrete activator \( (u_1) \) profile for the Schnakenberg reaction kinetics on a domain with spatially linear evolution at times 0, 580, 1000, 1500 and 2000. The substrate \( (u_2) \) profile is omitted as they are out of phase with those of the activator. For parameter values see Table 3. The results are computed using the evolving domain formulation (6.11) with a uniform timestep and initial mesh. We observe the formation of a half spot which reorients to a single spot positioned in the centre of the domain. As the domain contracts this single spot is annihilated with the domain at end time exhibiting no patterns.

Figure 3. Snapshots of the discrete activator \( (u_1) \) profile for the Schnakenberg reaction kinetics on a domain with spatially nonlinear evolution at times 0, 590, 1000, 1750 and 2000. For parameter values see Table 3. The results are computed using the reference domain formulation (6.2) with a uniform timestep and mesh. Although the evolution of the domain boundary is identical to the spatially linear case, the pattern transitions observed are markedly different with the formation of a half spot that splits into two half spots which are annihilated as the domain contracts to leave a final domain with no patterns.
FIGURE 4. Snapshots of the discrete activator \( u_1 \) profile for the Schnakenberg reaction kinetics on the reference domain and mapped to the evolving domain corresponding to system (6.2) and nonlinear domain evolution of the form (7.5). For parameter values see text. We see that spots form and increase in number (via splitting) as the domain grows and decrease in number (via annihilation) as the domain contracts. The spots appear to possess a common amplitude and maintain a relatively uniform separation distance on the evolving domain.

component model. We first consider a fixed domain, to illustrate both the qualitatively different solution behaviour to the 2 component case and that our method is readily applicable to multicomponent RDSs posed on fixed domains.

7.5. Definition (Global and local inhibition kinetics [20]). The following model is comprised of a single self-enhancing activator \( u_1 \) antagonised by global (fast diffusing) and local (slow diffusing) inhibitors; \( u_2 \) and \( u_3 \) respectively:

\[
\begin{align*}
    f_1 (u_1, u_2, u_3) &= \gamma \left( \frac{s(u_1^2 + b_1)}{u_2(1 + s_3 u_3)} - r_1 u_1 \right), \\
    f_2 (u_1, u_2, u_3) &= \gamma \left( s u_1^2 - r_2 u_2 \right), \\
    f_3 (u_1, u_2, u_3) &= \gamma \left( r_3 u_1 - r_3 u_3 \right),
\end{align*}
\]

(7.6)
where \( 0 \leq s, b_1, r_1, s_3, r_2, r_3, \gamma < \infty \). We select the set of parameter values given in Tables 4 and 5. We take the domain to be the square \( \Omega = [-1, 1]^2 \). Snapshots of the discrete solutions are reported in Figure 5. An initial 4 spot pattern forms with a rapid transition to a 2 spot solution. The 2 spots then move around the domain boundary in a travelling wave like fashion. As expected from intuition, the activator \( u_1 \) and local inhibitor \( u_3 \) concentrations are significantly more localised than the global inhibitor concentration \( u_3 \). For details on the behaviour of 3 component systems (on fixed domains) and heuristic explanations of the observed behaviour we refer to [20]. The behaviour is markedly different to the 2-species case. No spatially inhomogeneous steady state is observed. None of the species are in or out of phase with spatial peaks of the global inhibitor travelling slightly ahead of spatial peaks of the activator which travels ahead of the spatial peaks of the local inhibitor.

We now consider the same system posed on an evolving domain. Figure 6 shows snapshots of the evolution on a domain with growth of the form (7.2) and parameter values as given in Tables 4 and 6. Broadly speaking similar behaviour to the 2 component case is observed with the patterning mode (number of spots) generally increasing as the domain grows and decreasing as the domain contracts. The initial pattern is a 2 peak pattern that exhibits travelling wave behaviour similar to the fixed case. After the domain has grown sufficiently large new peaks appear either via splitting of existing peaks or peak insertion. When multiple peak patterns are present the behaviour is much more complicated than the two component case, the peaks travel around the domain and can collide leading to peak-merging or when peaks are in close proximity peak-annihilation, as reported in Figure 7. This behaviour of peak-merging and annihilation was observed previously by Venkataraman et al. [30] for 2 component systems, the novelty in the 3 component case is that this behaviour is observed even as the domain grows. This is of interest as with this specific 3 component system domain growth (contraction) does not lead to a monotonic increase (decrease) in the number of peaks. Our observations of these novel behaviours of 3 component systems on evolving domains is to the best of our knowledge new and definitely warrants further investigation.

### Table 4

| \( D_1 \) | \( D_2 \) | \( D_3 \) | \( \gamma \) | \( s \) | \( s_3 \) | \( r_1 \) | \( r_2 \) | \( r_3 \) | \( b_1 \) |
|---------|---------|---------|--------|-----|-----|-----|-----|-----|-----|
| 1.0     | 100     | 0.01    | \( 10^4 \) | 0.005 | 0.8 | 0.005 | 0.008 | 0.001 | 0.01 |

**Table 4.** Parameter values for numerical experiments with the 3 component kinetics.

| \( T \) | \( \tau \) | DOFs |
|-------|-------|------|
| 5     | \( 10^{-3} \) | 8321 |

**Table 5.** Numerical parameter values for experiments with the 3 component kinetics on a fixed domain.

| \( \kappa \) | \( T \) | \( \tau \) | DOFs |
|-------|-------|-------|------|
| 4     | 100   | \( 10^{-3} \) | 8321 |

**Table 6.** Parameter values for numerical experiments with the 3 component kinetics on an evolving domain.
Figure 5. Snapshots of the discrete activator $u_1$ (left), discrete global inhibitor $u_2$ (middle) and discrete local inhibitor $u_3$ (right) for the 3 component system (7.6) on a fixed domain at times 0.65, 1, 1.5, 2, 3.5 and 5. The colour (grey-scale) legend to the right of each column indicates the numerical range of each component during the experiment. The global inhibitor concentration is less spatially localised than the activator and local inhibitor concentration. We observe travelling wave like solutions. An initial 4 peak solution forms, subsequently 2 peaks are annihilated leaving a 2 peak solution which travels around the boundary of the domain for the remainder of the evolution.
Figure 6. Snapshots of the discrete activator $u_1$ (top), discrete global inhibitor $u_2$ (middle) and discrete local inhibitor $u_3$ (bottom) for the 3 component system (7.6) on a domain with spatially linear evolution at times 0.5, 1, 2, 3, 4, 5, 6, 7, 8, 9 and 10 reading clockwise. The colour (grey-scale) legend above each row indicates the numerical range of each component during the experiment. Generally more peaks are observed on larger domains, however the behaviour is much richer than the 2 component case with the travelling wave like nature of the solutions leading to peak collisions which result in spot merging or peak annihilation when spots move into close proximity.
Figure 7. Snapshots of the activator profiles of the 3 component system on the evolving domain between $t = 4.75$ and $t = 4.8$ at intervals of 0.01. We observe peak merging, with the two peaks in the bottom left hand corner (within the dashed oval) merging and peak annihilation with the right most of the two peaks contained in the dashed rectangle being annihilated. Note the mode number of the pattern (number of spots) at $t = 4.8$ is less than at $t = 4.75$.

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