THE IDENTIFICATION OF SPACE-TIME DISTRIBUTED PARAMETERS IN REACTION-DIFFUSION SYSTEMS

MARCUS R. GARVIE* AND C. TRENCHEA†

Abstract. We consider a general methodology for parameter identification in systems of reaction-diffusion equations. To demonstrate the method we focus on the classic Gierer-Meinhardt reaction-diffusion system. The original Gierer-Meinhardt model [A. Gierer and H. Meinhardt, *Kybernetik*, 12 (1972), pp. 30-39] was formulated with constant parameters and has been used as a prototype system for investigating pattern formation in developmental biology. In our paper the parameters are extended in space and time and used as distributed control variables. The methodology employs PDE-constrained optimization in the context of image-driven spatiotemporal pattern formation. We prove the existence of optimal solutions, derive an optimality system, and determine the optimal solutions. The results of some numerical experiments in 2-D are presented using the finite element method, which illustrates the convergence of a variable-step gradient algorithm for finding the optimal parameters of the system.

Key words. optimal control theory, parameter identification, reaction-diffusion equations, image-driven optimization, variable-step gradient algorithm, finite element method

AMS subject classifications. 49J20, 93B30, 35K57

1. Introduction. Many processes in the applied sciences can be adequately modeled by partial differential equations [13]. However, it is not always possible to measure or calculate the model parameters with the necessary accuracy, particularly in living organisms. In these cases mathematical techniques for estimating model parameters become important. Parameter estimation is also an important technique for identifying redundant parameters (and hence the key parameters) in complex systems with many parameters. The need to identify parameters in evolution equations arises in many disciplines, including biology, physics, engineering, and chemistry. A considerable amount of research has been devoted to the development of computational methods for estimating parameters in such equations (see, for example [3, 2, 1, 4, 5, 9, 12, 19, 34] and the references therein). The typical procedure involves integrating the evolution equation to obtain a simulation result that is compared to an observed data set, and then the application of least squares techniques to minimize a cost functional with respect to parameters in an admissible set [1].

In this paper we consider a methodology for parameter identification in nonlinear reaction-diffusion (RD) equations. There are relatively few works that focus on parameter identification for RD equations, which is a fertile and growing area of research with many applications, for example, population dynamics [10, 22], synaptic transmission at a neuromuscular junction [8], color negative film development [14], chemotaxis [11], epidemiology [21], and brain tumor growth [20].

Traditional studies of RD equations have focussed on models with spatially homogeneous parameters. In reality, parameters often operate in spatially heterogeneous environments. A number of previous authors have considered RD models with spatially varying parameters (see, for example [6, 24, 27, 28]), but to our knowledge none allow the parameters to vary freely in time. By relaxing this assumption, and allowing

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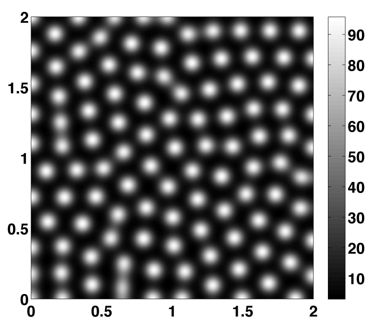
the parameters to vary in space and time, we develop an image-driven methodology for parameter identification in RD equations with broad applicability.

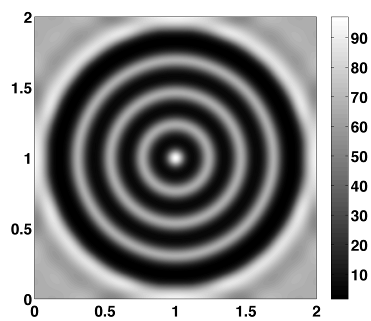
For concreteness, we illustrate our method by considering the identification problem for the two-component activator-inhibitor system of RD equations introduced by Gierer and Meinhardt [17] for pattern formation. The original formulation has fixed parameter values. We consider the more general situation where two key parameters, μ and α, depend on space x and time t. In non-dimensional form [27] the RD system has the following form

$$\begin{cases} \frac{\partial u}{\partial t} = D_u \Delta u + \frac{ru^2}{v} - \mu(x,t)u + r, \\ \frac{\partial v}{\partial t} = D_v \Delta v + ru^2 - \alpha(x,t)v, \end{cases} \tag{1.1}$$

with non-negative parameters r, D_u, and D_v, and non-negative morphogen concentrations $u(x,t)$ and $v(x,t)$. Δ denotes the standard Laplacian operator in two space dimensions.



(a)



(b)

Fig. 1.1: Numerical solutions u of (1.1) at time $T = 500$ with $D_v = 0.27$, $D_u = 9.45 \times 10^{-4}$, $r = 0.001$, $\alpha = 100$, with (a) $\mu = 2.5$, and (b) $\mu = 2.5$ within a circle of radius 0.9, centre $(1,1)$, and $\mu = 1.5$ elsewhere. Spatial discretization step $= 0.01$. An IMEX Galerkin finite element method with piecewise linear continuous basis functions was employed with first and second order time-stepping schemes 1-SBDF and 2-SBDF [30], with time steps 1×10^{-8} and 0.01 respectively. Homogeneous Neumann boundary conditions were employed. Initial data: u_0 and v_0 small random perturbations ($\pm 10\%$) of the steady state solutions.

When the parameters in the Gierer-Meinhardt model are appropriately chosen, the mechanism of 'diffusion induced instability', or Turing mechanism [33], leads to morphogen concentrations with characteristic regular spacing of peaks and troughs (a pattern) [17]. When the parameters μ and α are allowed to vary in space it has been shown that this increases the range and complexity of possible patterns [28]. Typical numerical solutions of the Gierer-Meinhardt system (1.1) for spatially homogeneous and inhomogeneous parameters are shown in Figures 1.1(a)-1.1(b).

We comment that the Gierer-Meinhardt model is not based on real kinetics and is used here for the purpose of illustrating our methodology for parameter identification in nonlinear RD equations, and thus no biological implications of our results should be made. The methodology outlined in our paper employs a PDE-constrained optimization procedure in the context of image-driven spatiotemporal pattern formation. The remainder of the paper has the following structure. In Section 2 the well-posedness of the direct problem is discussed, while in Section 3 a cost functional is defined that allows us to setup the inverse problem. In Section 4 we prove the existence of optimal solutions, derive an optimality system, and determine optimal solutions. In Section 5 the results of a numerical experiment is presented, which illustrates the convergence of a variable-step gradient algorithm for finding optimal parameters. Finally, in Section 6 we make some conclusions.

2. Well-posedness of the direct problem. Before stating the well-posedness result for the Gierer-Meinhardt model we need to establish the formal setting and restate the RD system with appropriate initial and boundary conditions. Let Ω be a bounded and open subset of $\mathbb{R}^d$, $d \leq 2$, and $Q := \Omega \times (0,T)$ be the space-time cylinder. The direct problem is formulated as follows:

Find the morphogen concentrations $u(x,t)$ and $v(x,t)$ such that

$$\frac{\partial u}{\partial t} = D_u \Delta u + \frac{ru^2}{v} - \mu(x,t)u + r \quad \text{in} \quad Q, \tag{2.1a}$$

$$\frac{\partial v}{\partial t} = D_v \Delta v + ru^2 - \alpha(x,t)v \quad \text{in} \quad Q, \tag{2.1b}$$

$$u(x,0) = u_0(x), \qquad v(x,0) = v_0(x), \quad x \in \Omega \tag{2.1c}$$

$$\frac{\partial u}{\partial \nu} = \frac{\partial v}{\partial \nu} = 0 \quad \text{on} \quad \partial\Omega \times (0,T), \tag{2.1d}$$

where the fixed parameters r, D_u, and D_v are non-negative, and $u(x,t)$ and $v(x,t)$ are the morphogen concentrations defined for $(x,t) \in Q$. D_u and D_v are the diffusion coefficients of u and v respectively, $\Delta = \sum_{i=1}^d \partial^2/\partial x_i^2$ denotes the standard Laplacian operator in $d \leq 2$ space dimensions, and ν denotes the outward normal to $\partial\Omega$, the boundary of Ω. We assume that $\mu(x,t)$ and $\alpha(x,t)$ are bounded, Lipschitz continuous functions on Q, which we denote by $\mu, \alpha \in \mathrm{Lip}\,(Q)$, belonging to the set of admissible parameters:

$$U_{ad} := \Big\{ \{\mu, \alpha\} : \mu, \alpha \in \mathrm{Lip}(Q), 0 \leq \mu(x,t) \leq \mu_1, 0 \leq \alpha(x,t) \leq \alpha_1 \Big\}, \tag{2.2}$$

for all $(x,t) \in Q$ and numbers $\mu_1, \alpha_1 \in \mathbb{R}$. We assume zero flux of the morphogen concentrations across the boundary and that the initial concentrations, $u_0(x)$, $v_0(x) \in C(\overline{\Omega})$, are bounded and nonnegative. It will be convenient to denote the vector of reaction kinetics by $\mathbf{f}(\mathbf{u}) := (f(\mathbf{u}), g(\mathbf{u}))^T$, where $\mathbf{u} := (u,v)^T$.

THEOREM 2.1. *Let $\mu, \alpha \in \mathrm{Lip}(Q)$ and $u_0(x), v_0(x) \in C(\overline{\Omega})$. Furthermore, assume that the initial data $(u_0(x), v_0(x))$ is in $[0,\infty)^2$ for all (or almost every) $x \in \Omega$. Then there exists a unique nonnegative classical solution of the Gierer-Meinhardt RD system* (2.1a)-(2.1d) *for all $(x,t) \in \Omega \times [0,\infty)$.*

Proof. The existence of a unique global classical solution of the system (2.1a)-(2.1d) follows from [29]. To prove the nonnegativity of solutions observe that the reaction kinetics satisfy

$$f(0,v),\ g(u,0) \geq 0 \quad \text{for all } u,v \geq 0,$$

and the initial data $(u_0(x), v_0(x))$ is in $[0,\infty)^2$ for all (or almost every) $x \in \Omega$. Thus by a maximum principle (see e.g., [31, Lemma 14.20]) the solution $(u(x,t), v(x,t))$ lies in $[0,\infty)^2$ for all $x \in \Omega$ and for all $t > 0$ for which the solution of (2.1a)-(2.1d) exists. In other words $[0,\infty)^2$ is positively invariant for the system. ∎

3. Setup of the inverse problem. For the identification or inverse problem we are given possibly perturbed measurements $(\overline{u}, \overline{v})$ corresponding to the state variables (u, v) and we must determine μ, α such that $(u_{\mu,\alpha}, v_{\mu,\alpha})$ best approximate $(\overline{u}, \overline{v})$.

For given $T > 0$, $u_0, v_0 \in C(\overline{\Omega})$, and $\overline{u}, \overline{v} \in L^2(Q)$ (not necessarily a solution of (2.1a)-(2.1d)), the least-squares approach leads to the minimization problem:

(**P**) Find $(\mu^*, \alpha^*) \in U_{ad}$ such that

$$J(\mu^*, \alpha^*) = \inf_{\mu,\alpha \in U_{ad}} J(\mu, \alpha),$$

where the cost functional J is defined by:

$$\begin{aligned} J(\mu, \alpha) &= \frac{1}{2} \int_0^T\!\!\int_\Omega \left(\beta_1 |u_{\mu,\alpha} - \overline{u}|^2 + \beta_2 |v_{\mu,\alpha} - \overline{v}|^2\right) dx dt \\ &\quad + \frac{1}{2} \int_\Omega \left(\gamma_1 |u_{\mu,\alpha}(x,T) - \overline{u}(x,T)|^2 + \gamma_2 |v_{\mu,\alpha}(x,T) - \overline{v}(x,T)|^2\right) dx, \end{aligned} \tag{3.1}$$

with $(u_{\mu,\alpha}, v_{\mu,\alpha})$ satisfying (2.1a)-(2.1d).

4. The minimization problem.

4.1. Existence of an optimal solution. We prove the existence of an optimal solution of the minimization problem (**P**) when Ω is an open bounded domain with Lipschitz continuous boundary $\partial\Omega$. We denote the usual $L^2(\Omega)$ norm by $\|\cdot\|$.

PROPOSITION 4.1. *Given $u_0, v_0 \in C(\overline{\Omega})$, and $\overline{u}, \overline{v} \in L^2(Q)$, there exists a solution $\mu^*, \alpha^* \in U_{ad}$ and $(u^*, v^*) \in C([0,T]; L^2(\Omega)^2) \cap L^2(0,T; H^1(\Omega)^2)$ of the minimization problem* (**P**).

Proof. Let $(\mu^n, \alpha^n, u^n \equiv u_{\mu^n,\alpha^n}, v^n \equiv v_{\mu^n,\alpha^n})$ be a minimizing sequence to (**P**), i.e.,

$$\begin{aligned} d = \inf_{\mu,\alpha \in U_{ad}} J(\mu, \alpha) &\le \int_0^T \left(\frac{\beta_1}{2} \|u^n - \overline{u}\|^2 + \frac{\beta_2}{2} \|v^n - \overline{v}\|^2\right) dt \\ &\quad + \frac{\gamma_1}{2} \|u^n(T) - \overline{u}(T)\|^2 + \frac{\gamma_2}{2} \|v^n(T) - \overline{v}(T)\|^2 < d + \frac{1}{n}. \end{aligned} \tag{4.1}$$

This implies that u^n, v^n are bounded in $L^2(Q)$ and recall that by (2.2) μ^n, α^n are bounded in $C(\overline{Q})$. Using energy-type estimates we will show that the corresponding solution (u^n, v^n) is bounded in $C([0,T]; L^2(\Omega)^2) \cap L^2(0,T; H^1(\Omega)^2)$. More precisely, consider the system (2.1a)-(2.1b) with the state variables (u^n, v^n) and coefficients (μ^n, α^n). Recall that in 2 dimensions we have (see e.g. [26]) by the Gagliardo-Nirenberg inequality

$$\|w\|_{L^4(\Omega)} \le C \|w\|_{L^2(\Omega)}^{1/2} \|w\|_{H^1(\Omega)}^{1/2} \qquad \forall w \in H^1(\Omega). \tag{4.2}$$

Multiplying the first equation in (2.1a)-(2.1b) by u^n and the second by v^n we obtain after some calculations

$$\begin{aligned} &\frac{d}{dt}\left(\|u^n(t)\|^2 + \|v^n(t)\|^2\right) + D_u \|\nabla u^n\|^2 + D_v \|\nabla v^n\|^2 \\ &\quad \le C\left(\|u^n\|^2 (1 + \|u^n\|^2) + \|v^n\|^2 (1 + \|v^n\|^2)\right), \end{aligned}$$

where by C we denote a generic constant that is independent of n.

Using (4.1), the Grönwall lemma, the Aubin lemma (see e.g. [23]) and the Arzelà-Ascoli theorem we can extract subsequences satisfying

$$
\begin{aligned}
&\mu^n \to \mu^*, \alpha^n \to \alpha^* && \text{in } C(\overline{Q}),\\
&u^n \to u^*, v^n \to v^* && \text{weakly in } L^2(0,T;H^1(\Omega))\cap\\
& && H^1(0,T;(H^1(\Omega))') \text{ and strongly in}\\
& && L^2(0,T;L^2(\Omega)),\\
&u^n \to u^*, v^n \to v^* && \text{weak-star in } L^\infty(0,T;L^2(\Omega)),\\
&u^n(\cdot,T)\to u^*(\cdot,T), v^n(\cdot,T)\to v^*(\cdot,T) && \text{weakly in } L^2(\Omega).
\end{aligned}
\tag{4.3}
$$

By the lower weak semicontinuity of the functional (3.1) we have

$$
J(\mu^*,\alpha^*) \le \liminf_{n\to\infty} J(\mu^n,\alpha^n). \tag{4.4}
$$

Using the weak and strong convergence results in (4.3), we pass to the limit inside the linear and nonlinear terms in (2.1a)-(2.1b) to show that $(u^*, v^*, \mu^*, \alpha^*)$ is a solution to (2.1a)-(2.1b), which by (4.4) implies that $(\mu^*, \alpha^*, u^*, v^*)$ is an optimal solution to problem $(\mathbf{P})$. ∎

4.2. First-order necessary conditions. We derive the first-order necessary conditions associated with the optimal control problem $(\mathbf{P})$. If the Gâteaux derivative of the functional exists, then the optimal solution must satisfy this standard first-order necessary condition (see, e.g., [32]).

LEMMA 4.2. *Let $u_0, v_0 \in C(\overline{\Omega})$. If $(u^*, v^*, \mu^*, \alpha^*)$ is an optimal solution and the functional $J(\mu^*,\alpha^*)$ is Gâteaux differentiable, then the necessary condition for (μ^*,α^*) to be a minimizer of $J(\mu^*,\alpha^*)$ is*

$$
\frac{DJ(\mu^*,\alpha^*)}{D(\mu,\alpha)} \cdot (\mu-\mu^*, \alpha-\alpha^*) \ge 0 \quad \forall (\mu,\alpha) \in U_{ad}.
$$

It is clear that for $(\mu,\alpha) \in U_{ad}$ the solution (u,v) of (2.1a) - (2.1d) is classical and hence weak. It is convenient to work in the topology of $L^2(0,T;H^1(\Omega))$, which allows us to use well-known results. We recall that the solution of (2.1a)-(2.1b) defines a mapping $u = u_{\mu,\alpha}, v = v_{\mu,\alpha}$ from U_{ad} to $L^2(0,T;H^1(\Omega))$, which is Gâteaux differentiable and thus Lemma 4.2 can be applied.

LEMMA 4.3. *Let $u_0, v_0 \in C(\overline{\Omega})$. The map $(\mu,\alpha) \mapsto (u_{\mu,\alpha}, v_{\mu,\alpha})$ from U_{ad} to $L^2(0,T;H^1(\Omega)^2)$, defined as the solution of (2.1a)-(2.1d), has a Gâteaux derivative in every direction $(\widehat{\mu},\widehat{\alpha})$ in U_{ad}. Furthermore, $(\widehat{u},\widehat{v}) = (\frac{du}{d(\mu,\alpha)}, \frac{dv}{d(\mu,\alpha)}) \cdot (\widehat{\mu},\widehat{\alpha})$ is the solution of the problem*

$$
\begin{aligned}
\widehat{u}_t - D_u\Delta\widehat{u} &= r\frac{2u\widehat{u}v + u^2\widehat{v}}{v^2} - \widehat{\mu}u - \mu\widehat{u},\\
\widehat{v}_t - D_v\Delta\widehat{v} &= 2ru\widehat{u} - \widehat{\alpha}v - \alpha\widehat{v},
\end{aligned}
\tag{4.5}
$$

augmented with zero initial conditions and the homogeneous Neumann boundary conditions.

Proof. Let (μ,α), $(\widehat{\mu},\widehat{\alpha})$ be given in U_{ad}. We denote by $(u_\lambda, v_\lambda) = (u_{\mu+\lambda\widehat{\mu},\alpha+\lambda\widehat{\alpha}}, v_{\mu+\lambda\widehat{\mu},\alpha+\lambda\widehat{\alpha}})$ and $(u,v) = (u_{\mu,\alpha}, v_{\mu,\alpha})$ the solutions of (2.1a)-(2.1b) with coefficients $(\mu+\lambda\widehat{\mu}, \alpha+\lambda\widehat{\alpha})$ and (μ,α), respectively. Subtracting these two systems we obtain

$$
\begin{aligned}
(u_\lambda - u)_t - D_u\Delta(u_\lambda - u) &= r\frac{(u_\lambda^2 - u^2)v + u^2(v - v_\lambda)}{v_\lambda v} - \lambda\widehat{\mu}u_\lambda - \mu(u_\lambda - u),\\
(v_\lambda - v)_t - D_v\Delta(v_\lambda - v) &= r(u_\lambda^2 - u^2) - \lambda\widehat{\alpha}v_\lambda - \alpha(v_\lambda - v),
\end{aligned}
\tag{4.6}
$$

augmented with zero initial conditions and the homogeneous Neumann boundary conditions. After multiplying the first equation by $u_\lambda - u$, the second by $v_\lambda - v$, and adding, we have

$$\begin{aligned}
&\frac{d}{2dt}\left(\|u_\lambda - u\|^2 + \|v_\lambda - v\|^2\right) + D_u\|\nabla(u_\lambda - u)\|^2 + D_v\|\nabla(v_\lambda - v)\|^2 \\
&= \int_\Omega (u_\lambda - u)^2\left(r\frac{u_\lambda + u}{v_\lambda} - \mu\right)dx + r\int_\Omega (u_\lambda - u)(v - v_\lambda)\frac{u^2}{v_\lambda v}dx - \lambda\int_\Omega \widehat{\mu}u_\lambda(u_\lambda - u)dx \\
&\quad - \int_\Omega \alpha(v_\lambda - v)^2dx + r\int_\Omega (u_\lambda - u)(v_\lambda - v)(u_\lambda + u)dx - \lambda\int_\Omega \widehat{\alpha}v_\lambda(v_\lambda - v)dx \\
&\le \frac{r}{v_{\inf}}\|u_\lambda + u\|\|u_\lambda - u\|^2_{L^4} + \frac{r}{v_{\inf}^2}\|u_\lambda - u\|_{L^4}\|v_\lambda - v\|_{L^4}\|u\|^2_{L^4} + \lambda\|\widehat{\mu}\|\|u_\lambda\|_{L^4}\|u_\lambda - u\|_{L^4} \\
&\quad + r\|u_\lambda - u\|_{L^4}\|v_\lambda - v\|_{L^4}\|u_\lambda + u\| + \lambda\|\widehat{\alpha}\|\|v_\lambda\|_{L^4}\|v_\lambda - v\|_{L^4},
\end{aligned}$$

where $v_{\inf} := \inf v > 0$ for all $(x,t) \in \Omega \times [0,\infty)$. Here we use (4.2) in the form

$$\|u\|_{L^4} \le C\|u\|^{\frac12}\left(\|u\| + \|\nabla u\|\right)^{\frac12} = C\left(\|u\|^2 + \|u\|\|\nabla u\|\right)^{\frac12} \le C\left(\|u\| + \|u\|^{\frac12}\|\nabla u\|^{\frac12}\right),$$

to obtain

$$\begin{aligned}
&\frac{d}{dt}\left(\|u_\lambda - u\|^2 + \|v_\lambda - v\|^2\right) + D_u\|\nabla(u_\lambda - u)\|^2 + D_v\|\nabla(v_\lambda - v)\|^2 \\
&\quad \le \|u_\lambda - u\|^2 C\left(\|u\|^4 + \|u\|^2\|\nabla u\|^2 + \|u_\lambda\|^2 + \|u\|^2 + \|\nabla u_\lambda\|^2 + 1\right) \\
&\qquad + \|v_\lambda - v\|^2 C\left(\|u\|^4 + \|u\|^2\|\nabla u\|^2 + \|u_\lambda\|^2 + \|v_\lambda\|^2 + \|\nabla v_\lambda\|^2 + \|u\|^2 + 1\right) \\
&\qquad + \lambda^2 C\left(\|u_\lambda\|^2 + \|\widehat{\mu}\|^2 + \|\widehat{\alpha}\|^2\|v_\lambda\|^2 + \|\widehat{\alpha}\|^2\right).
\end{aligned}$$

Now (4.3) and the Grönwall lemma yield

$$\begin{aligned}
&\|u_\lambda(t) - u(t)\|^2 + \|v_\lambda(t) - v(t)\|^2 + \int_0^t \left(D_u\|\nabla(u_\lambda - u)(\tau)\|^2 + D_v\|\nabla(v_\lambda - v)(\tau)\|^2\right)d\tau \\
&\le C\lambda^2\int_0^T (\|\widehat{\mu}(t)\|^2 + \|\widehat{\alpha}(t)\|^2)dt.
\end{aligned}\tag{4.7}$$

We need to prove that

$$\lim_{\lambda\to 0}\frac{\|(u_\lambda - u - \lambda\widehat{u}, v_\lambda - v - \lambda\widehat{v})\|_{L^2(0,T;H^1(\Omega)^2)}}{|\lambda|} = 0. \tag{4.8}$$

Set $\breve{u} = u_\lambda - u - \lambda\widehat{u}$, $\breve{v} = v_\lambda - v - \lambda\widehat{v}$ so then by (4.5) and (4.6) we see that $(\breve{u}, \breve{v})$ satisfies

$$\begin{aligned}
&\breve{u}_t - D_u\Delta\breve{u} \\
&= r\frac{\breve{u}(u_\lambda + u)v^2 + \lambda\widehat{u}v[(u_\lambda - u)v + 2u(v - v_\lambda)] + u^2v\breve{v} + \lambda u^2\widehat{v}[v - v_\lambda]}{v^2 v_\lambda} - \lambda\widehat{\mu}(u_\lambda - u) - \mu\breve{u}, \\
&\breve{v}_t - D_v\Delta\breve{v} = r\left[\breve{u}(u_\lambda + u) + \lambda\widehat{u}(u_\lambda - u)\right] - \lambda\widehat{\alpha}(v_\lambda - v) - \alpha\breve{v}.
\end{aligned}$$

Now we multiply these equations by $\breve{u}$ and $\breve{v}$ respectively, and add to get

$$
\begin{aligned}
&\frac{d}{2dt}\left(\|\breve{u}\|^2+\|\breve{v}\|^2\right)+D_u\|\nabla\breve{u}\|^2+D_v\|\nabla\breve{v}\|^2\\
&=r\int_\Omega \breve{u}^2\frac{(u_\lambda+u)}{v_\lambda}+r\lambda\int_\Omega \breve{u}(u_\lambda-u)\frac{\widehat{u}}{v_\lambda}+2r\lambda\int_\Omega \breve{u}(v-v_\lambda)\frac{u\widehat{u}}{vv_\lambda}+r\int_\Omega \breve{u}\breve{v}\frac{u^2}{vv_\lambda}\\
&\qquad+r\lambda\int_\Omega \breve{u}[v-v_\lambda]\frac{u^2\widehat{v}}{v^2v_\lambda}-\lambda\int_\Omega \breve{u}\widehat{\mu}(u_\lambda-u)-\int_\Omega \mu(x,t)\breve{u}^2\\
&\qquad+r\int_\Omega \breve{u}\breve{v}(u_\lambda+u)+\lambda r\int_\Omega \breve{v}(u_\lambda-u)\widehat{u}-\lambda\int_\Omega \breve{v}(v_\lambda-v)\widehat{\alpha}-\int_\Omega \alpha(x,t)\breve{v}^2\\
&\le\frac{D_u}{2}\|\nabla\breve{u}\|^2+\frac{D_v}{2}\|\nabla\breve{v}\|^2\\
&+C\left(\|\breve{u}\|^2+\|\breve{v}\|^2\right)\left(\|u_\lambda\|^2+\|u\|^2+\lambda^2\|u_\lambda-u\|^2\|\widehat{u}\|^2+\|u\|_{L^4}\|v\|_{L^4}+\|u\|_{L^4}^4+1\right)\\
&+\lambda^2\left(\|u_\lambda-u\|^2+\|\nabla(u_\lambda-u)\|^2+\|v-v_\lambda\|^2+\|\nabla(v-v_\lambda)\|^2\right)\\
&\times\left(\|\widehat{u}\|^2+\|\widehat{\mu}\|^2+\|\widehat{\alpha}\|^2\right)+\lambda^2\|v_\lambda-v\|^2\|u\|_{L^4}^2\|\widehat{u}\|_{L^4}^2+\lambda^2\|\nabla(v_\lambda-v)\|^2\\
&+C\lambda\Big(\|\breve{u}\|\|v-v_\lambda\|+\|\breve{u}\|^{1/2}\|\nabla\breve{u}\|^{1/2}\|v-v_\lambda\|+\|\breve{u}\|\|v-v_\lambda\|^{1/2}\|\nabla(v-v_\lambda)\|^{1/2}\\
&+\|\breve{u}\|^{1/2}\|\nabla\breve{u}\|^{1/2}\|v-v_\lambda\|^{1/2}\|\nabla(v-v_\lambda)\|^{1/2}\Big)\|u\|_{C(\overline{Q})}^2\|\widehat{v}\|,
\end{aligned}
$$

and apply the Grönwall lemma

$$
\begin{aligned}
&\|\breve{u}(t)\|^2+\|\breve{v}(t)\|^2+\int_0^t\left(D_u\|\nabla\breve{u}(\tau)\|^2+D_v\|\nabla\breve{v}(\tau)\|^2\right)d\tau\\
&\le C\lambda^2\Big(\|u_\lambda(t)-u(t)\|^2+\|v_\lambda(t)-v(t)\|^2+\int_0^T\Big(D_u\|\nabla(u_\lambda-u)(t)\|^2+D_v\|\nabla(v_\lambda-v)(t)\|^2\Big)dt\Big).
\end{aligned}
$$

Finally from (4.7) we conclude that

$$
\|\breve{u}(t)\|^2+\|\breve{v}(t)\|^2+\int_0^T\left(D_u\|\nabla\breve{u}(t)\|^2+D_v\|\nabla\breve{v}(t)\|^2\right)dt\le C\lambda^4,
$$

which proves (4.8). □

The Gâteaux derivative provides useful information about the sensitivity of the system at a point (μ,α) in a particular direction $(\widehat{\mu},\widehat{\alpha})$, but complete information requires one to solve (4.5) for every possible direction $(\widehat{\mu},\widehat{\alpha})$. However, in order to minimize the functional we need only an integral over all these directions, which is obtained via the solution of an adjoint system.

Lemma 4.4. *Let $u_0,v_0\in C(\overline{\Omega})$, $(\widehat{\mu},\widehat{\alpha})\in U_{ad}$ and $(\widehat{u},\widehat{v})$ be defined through (4.5). For every $(F,G)\in L^2(0,T;L^2(\Omega)^2)$ we have*

$$
\int_0^T\int_\Omega\Big(F\widehat{u}+G\widehat{v}\Big)dxdt=-\int_\Omega(\mathsf{p}\widehat{u}+\mathsf{q}\widehat{v})\Big|_0^T dx-\int_0^T\int_\Omega(\widehat{\mu}u\mathsf{p}+\widehat{\alpha}v\mathsf{q})\,dxdt
$$

where $(\mathtt{p}, \mathtt{q})$ *is the solution of the adjoint problem*

$$
\begin{aligned}
&-\mathtt{p}_t - D_u\Delta\mathtt{p} - \left(2r\frac{u}{v} - \mu\right)\mathtt{p} - 2ru\mathtt{q} = F,\\
&-\mathtt{q}_t - D_v\Delta\mathtt{q} - r\frac{u^2}{v^2}\mathtt{p} + \alpha\mathtt{q} = G,\\
&\frac{\partial\mathtt{p}}{\partial\nu}(t,x) = \frac{\partial\mathtt{q}}{\partial\nu}(t,x) = 0, \quad x \in \partial\Omega,\\
&\mathtt{p}(T,x) = \mathtt{p}_T(x), \mathtt{q}(T,x) = \mathtt{q}_T(x), \quad x \in \Omega.
\end{aligned}
\tag{4.9}
$$

Proof. The left-hand side can be evaluated by (4.9) and (4.5) via integration by parts, which is justified by the regularity of the quantities involved:

$$
\begin{aligned}
&\int_0^T\int_\Omega \left(F\widehat{u} + G\widehat{v}\right)dxdt\\
&= \int_0^T\int_\Omega \left(-\mathtt{p}_t - D_u\Delta\mathtt{p} - \left(2r\frac{u}{v} - \mu\right)\mathtt{p} - 2ru\mathtt{q}\right)\widehat{u}\,dxdt\\
&\quad + \int_0^T\int_\Omega \left(-\mathtt{q}_t - D_v\Delta\mathtt{q} - r\frac{u^2}{v^2}\mathtt{p} + \alpha\mathtt{q}\right)\widehat{v}\,dxdt\\
&= \int_0^T\int_\Omega \left(\widehat{u}_t - D_u\Delta\widehat{u} - \left(2r\frac{u}{v} - \mu\right)\widehat{u} - r\frac{u^2}{v^2}\widehat{v}\right)\mathtt{p}\,dxdt\\
&\quad + \int_0^T\int_\Omega (\widehat{v}_t - D_v\Delta\widehat{v} + \alpha\widehat{v} - 2ru\widehat{u})\,\mathtt{q}\,dxdt - \int_\Omega (\mathtt{p}\widehat{u} + \mathtt{q}\widehat{v})\Big|_0^T dx\\
&= -\int_0^T\int_\Omega (\mathtt{p}\widehat{\mu}u + \mathtt{q}\widehat{\alpha}v)dxdt - \int_\Omega (\mathtt{p}\widehat{u} + \mathtt{q}\widehat{v})\Big|_0^T dx.
\end{aligned}
$$

□

Now we show that the optimal parameters μ^*, α^* are characterized in Lemma 4.2 by the solution of a particular adjoint system.

THEOREM 4.5. *Let* $(u^*, v^*, \alpha^*, \mu^*)$ *be an optimal solution to problem* $(\mathbf{P})$, $\overline{u}, \overline{v} \in C(\overline{\Omega})$, *and let* (p, q) *be the solution of the particular adjoint problem*

$$
\begin{aligned}
&-p_t - D_u\Delta p - \left(2r\frac{u^*}{v^*} - \mu\right)p - 2ru^*q = \beta_1(u^* - \overline{u}),\\
&-q_t - D_v\Delta q - r\frac{{u^*}^2}{{v^*}^2}p + \alpha q = \beta_2(v^* - \overline{v}),\\
&\frac{\partial p}{\partial\nu}(t,x) = 0, \frac{\partial p}{\partial\nu}(t,x) = 0, \quad x \in \partial\Omega,\\
&p(T,x) = \gamma_1(u^*(T,x) - \overline{u}(T,x)), q(T,x) = \gamma_2(v^*(T,x) - \overline{v}(T,x)), \quad x \in \Omega.
\end{aligned}
\tag{4.10}
$$

Then we have

$$
\int_0^T\int_\Omega -u^*p(\mu - \mu^*) - v^*q(\alpha - \alpha^*)dxdt \geq 0 \qquad \forall(\mu, \alpha) \in U_{ad}.
\tag{4.11}
$$

Proof. Let (μ^*, α^*) and (u^*, v^*) be an optimal solution of $(\mathbf{P})$. We compute the Gâteaux derivative of the cost functional $J(\mu^*, \alpha^*)$ in the direction of $(\widehat{\mu}, \widehat{\alpha})$. We have

$$\begin{aligned}
&\frac{DJ(\mu^*, \alpha^*)}{D\,(\mu, \alpha)} \cdot (\widehat{\mu}, \widehat{\alpha}) \\
&= \int_0^T \int_\Omega \beta_1 (u^* - \overline{u}) \left(\frac{du^*_{\mu^*,\alpha^*}}{d(\mu, \alpha)} \cdot (\widehat{\mu}, \widehat{\alpha}) \right) + \beta_2 (v^* - \overline{v}) \left(\frac{dv^*_{\mu^*,\alpha^*}}{d(\mu, \alpha)} \cdot (\widehat{\mu}, \widehat{\alpha}) \right) dxdt \\
&\quad + \gamma_1 \int_\Omega (u^*(T,x) - \overline{u}(T,x)) \left(\frac{du^*_{\mu^*,\alpha^*}}{d(\mu, \alpha)} \cdot (\widehat{\mu}, \widehat{\alpha}) \right) (T,x) dx \\
&\quad + \gamma_2 \int_\Omega (v^*(T,x) - \overline{v}(T,x)) \left(\frac{dv^*_{\mu^*,\alpha^*}}{d(\mu, \alpha)} (\widehat{\mu}, \widehat{\alpha}) \right) (T,x) dx \\
&= \int_0^T \int_\Omega (-\widehat{\mu} u^* p - \widehat{\alpha} v^* q)\, dxdt,
\end{aligned}$$

where $(\frac{du^*_{\mu^*,\alpha^*}}{d(\mu,\alpha)}, \frac{dv^*_{\mu^*,\alpha^*}}{d(\mu,\alpha)})$ is the solution of the sensitivity system (4.5). Now from the definition of optimality in problem $(\mathbf{P})$, as $(u^*, v^*, \mu^*, \alpha^*)$ is an optimal solution and the Gâteaux derivative of the functional exists, then from Lemma 4.4

$$\int_0^T \int_\Omega -u^* p(\mu - \mu^*) - v^* q(\alpha - \alpha^*) dxdt \geq 0 \qquad \forall (\mu, \alpha) \in U_{ad},$$

which concludes the proof. ∎

5. Numerical results. To illustrate the effectiveness of the image-driven PDE - constrained optimization procedure, we present numerical results in two space dimensions.

For the specific target functions $(\overline{u}, \overline{v})$ in our numerical simulations we chose the skin patterns of the Emperor Angelfish (*Pomacanthus imperator*). Our starting point prior to pre-processing of the image was a high resolution JPEG image [*,†], fitted into the square $[0, 2] \times [0, 2]$. The original image is initially cropped, which excludes the portion of the tail with no pattern and the background details. The cropped image is also used to define the domain Ω. The cropped image is then converted to gray scale and interpolated onto a fine irregular finite element mesh. This final image constitutes the target functions for the optimal control algorithm (for further details see [15]).

The spatial discretization of the state equations and adjoint equations were undertaken using a 'lumped mass', Galerkin finite element method with piecewise linear continuous basis functions. For the time discretization it is well-known that several popular time-stepping schemes for RD equations modeling pattern formation yield qualitatively poor results [30]. We therefore used a second order, 3-level, implicit-explicit (IMEX) scheme (2-SBDF) recommended by Ruuth in [30] as a good choice for most RD problems for pattern formation. IMEX schemes use an implicit discretization of the diffusion term, and an explicit discretization of the reaction terms. As the scheme 2-SBDF involves three time levels we need to 'kick-start' the approximation at the first time level, which we did using a first order IMEX scheme (1-SBDF) with a small time step [30]. The resulting sparse linear systems were solved in MATLAB (R2007a) using the GMRES iterative solver.

[*] 1050×750 (3.5in by 2.5in at 300ppi)

[†] Copyright Robert Fenner, `WetWebMedia.com`

To approximate the inverse problem we apply a variable-step gradient algorithm [7, 18, 16] yielding a sequence of discrete approximations $\{(u^k, v^k), (\mu^k, \alpha^k)\}_{k\in\mathbb{N}}$ to the optimal solutions (u^*, v^*) and optimal parameters (μ^*, α^*). The sensitivities of the system (2.1a)-(2.1b) and cost functional (3.1) with respect to the parameters (μ, α) are used to compute the Lagrange multipliers, satisfying the adjoint system that marches backward in time. The Lagrange multipliers are then used in the variable step gradient algorithm to minimize the cost functional. The implementation is straightforward, although computationally intensive. The bulk of the computational cost is in the backward-in-time solution of the adjoint system and the forward-in-time solution of the state system.

We used a nonuniform triangulation Ω^h of the angelfish domain Ω with 17,904 nodes and 35,280 triangles, and numerically solved the optimal control problem upto time $T = 10$ with uniform time steps $\Delta t = 1 \times 10^{-8}$ (1-SBDF) and $\Delta t = 0.01$ (2-SBDF). Figure 5.1 shows a snapshot at $T = 10$ of the optimal solution u, the target function $\bar{u}$, and the optimal parameters α and μ (see the caption for parameter values). For further details concerning the fully-discrete optimality system see Section 7.2 in the Appendix.

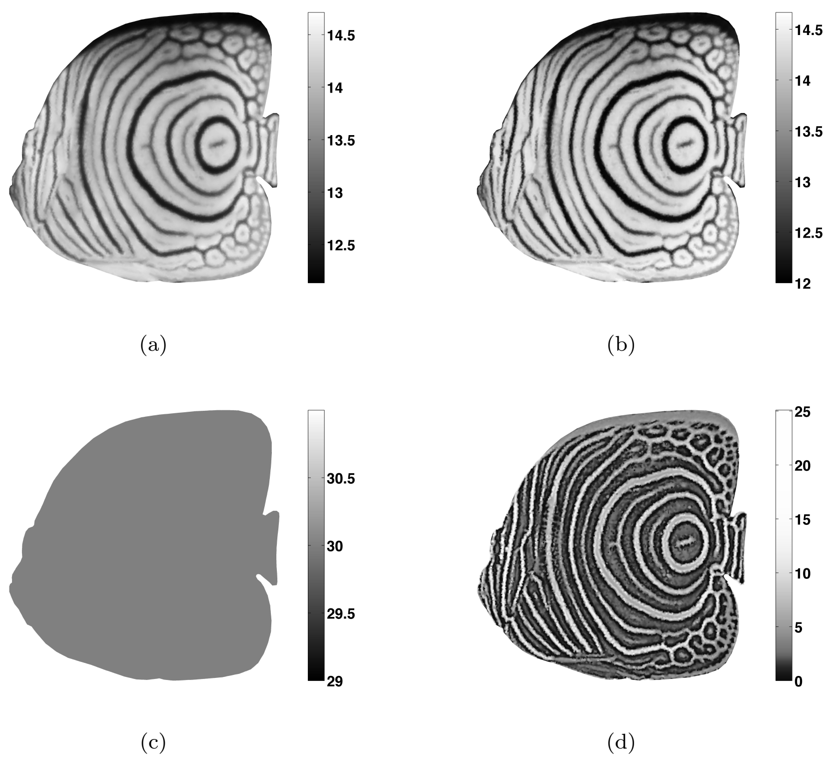


Fig. 5.1: (a) Optimal solution u, (b) stationary target function $\bar{u}$, (c) optimal parameter α, and (d) optimal parameter μ, at time $T = 10$. Parameter values: $D_u = D_v = 0.01$, $r = 10$, $\beta_1 = 0$, $\beta_2 = 0$, $\gamma_1 = 1$, $\gamma_2 = 0$, $\delta_1 = 1 \times 10^{-6}$, $\delta_2 = 1 \times 10^{-6}$. Initial data: $\mu = 3$, $\alpha = 30$, u_0 and v_0 small random perturbations ($\pm 10\%$) of the steady state solutions. Time steps: 1×10^{-8} (1-SBDF), 0.01 (2-SBDF). Mesh: 17904 nodes and 35280 triangles.

6. Conclusions. In this paper we outlined a general method for parameter identification in nonlinear reaction-diffusion equations based on a PDE-constrained image-driven optimization procedure (optimal control problem). For concreteness we focussed on the classic Gierer-Meinhardt reaction-diffusion system for pattern formation, with two distributed control parameters depending on space and time. For the target functions we employed a (pre-processed) image of a marine angelfish. The mathematical formulation, analysis, and numerical solution of the optimal control problem was presented. After undertaking the mathematical analysis of the optimal control problem, numerical solutions were obtained with the aid of a semi-implicit, Galerkin finite element method with piecewise linear continuous basis functions. The time-stepping procedure was based on a 2nd order, 3-level, implicit-explicit (IMEX) scheme. The numerical results illustrated the success of a variable step gradient algorithm to identify the parameters needed to drive the solution patterns of the Gierer-Meinhardt system close to the skin patterns of a marine angelfish. The potential biological applications of our methodology are discussed in a separate paper [15].

7. Appendix.

7.1. Modified cost functional. For computational convenience we modified the cost functional (3.1) to take into account the 'cost of control', which is a practical means of limiting the growth of the distributed control parameters:

$$
\begin{aligned}
J^{\delta_1,\delta_2}(\mu,\alpha) &= \frac{1}{2}\int_0^T\!\!\int_\Omega \left(\beta_1|u_{\mu,\alpha}-\overline{u}|^2+\beta_2|v_{\mu,\alpha}-\overline{v}|^2\right)dxdt \\
&+\frac{1}{2}\int_\Omega \left(\gamma_1|u_{\mu,\alpha}(x,T)-\overline{u}(x,T)|^2+\gamma_2|v_{\mu,\alpha}(x,T)-\overline{v}(x,T)|^2\right)dx, \\
&+\frac{1}{2}\int_0^T\!\!\int_\Omega \left(\delta_1\mu^2+\delta_2\alpha^2\right)dxdt.
\end{aligned}
\tag{7.1}
$$

The corresponding minimization problem becomes

(P) Find $(\mu^*,\alpha^*)\in U_{ad}$ such that

$$J^{\delta_1,\delta_2}(\mu^*,\alpha^*)=\inf_{\mu,\alpha\in U_{ad}} J^{\delta_1,\delta_2}(\mu,\alpha),$$

where the cost functional J^{δ_1,δ_2} is defined by (7.1), with $(u_{\mu,\alpha},v_{\mu,\alpha})$ satisfying (2.1a)-(2.1d).

It is straightforward to prove that Proposition 4.1 still holds, while the conclusion of Theorem 4.5 gives an explicit form for the optimal solution:

$$\mu^*=\frac{1}{\delta_1}u^*p, \qquad \alpha^*=\frac{1}{\delta_2}v^*q.$$

Here (p,q) is a solution to the adjoint problem (4.10).

7.2. Fully discrete optimality system. In order to construct stable finite element approximations, we introduce the following regularized version of (2.1a)-(2.1b):

$$
\begin{cases}
\frac{\partial u_\varepsilon}{\partial t}=D_u\Delta u_\varepsilon+\frac{ru_\varepsilon^2}{v_\varepsilon+\varepsilon u_\varepsilon^2+\varepsilon}-\mu(x,t)u_\varepsilon+r, \\
\frac{\partial v_\varepsilon}{\partial t}=D_v\Delta v_\varepsilon+\frac{ru_\varepsilon^2}{1+\varepsilon u_\varepsilon^2}-\alpha(x,t)v_\varepsilon,
\end{cases}
\tag{7.2}
$$

where ε is a small parameter. In subsequent calculations we drop the subscript of ε from u and v (and their discretized counterparts) for notational convenience. The global existence and uniqueness of the classical solutions of this regularized system follows in a straightforward manner from the theoretical framework of Morgan [25].

We introduce S^h, the standard Galerkin finite element space

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

Let $\{x_i\}_{i=0}^J$ be the set of nodes of the triangulation. 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 $j = 0, \dots J$. In order to define the finite dimensional weak forms of the reaction-diffusion system we define a discrete L^2 inner product on $C(\overline{\Omega})$ given by $(u, v)^h := \int_\Omega \pi^h(u(x)v(x))\, dx$, which approximates the usual L^2 inner product (u, v).

The fully discrete, first order scheme of system (7.2) for the first time step is given by the following problem: for $\mu_h^{(0)}, \alpha_h^{(0)} \in \mathrm{Lip}(\Omega)$ find $u_h^{(1)}, v_h^{(1)} \in S^h$ satisfying

$$\begin{aligned}
&\frac{1}{\Delta t}\left(u_h^{(1)} - u_h^{(0)}, \chi_h\right)^h + D_u\left(\nabla u_h^{(1)}, \nabla \chi_h\right) \\
&= \left(\frac{r|u_h^{(0)}|^2}{|v_h^{(0)}| + \varepsilon|u_h^{(0)}|^2 + \varepsilon} - \mu_h^{(0)} u_h^{(0)} + r, \chi_h\right)^h, \\
&\frac{1}{\Delta t}\left(v_h^{(1)} - v_h^{(0)}, \chi_h\right)^h + D_v\left(\nabla v_h^{(1)}, \nabla \chi_h\right) \\
&= \left(\frac{r|u_h^{(0)}|^2}{1 + \varepsilon|u_h^{(0)}|^2} - \alpha_h^{(0)} v_h^{(0)}, \chi_h\right)^h,
\end{aligned} \tag{7.3}$$

for all $\chi_h \in S^h$, with initial densities $u_h^{(0)} = \pi^h u_0(x)$, $v_h^{(0)} = \pi^h v_0(x)$. The fully discrete, second order scheme of system (7.2) is given by the following problem: for $\mu_h^{(n-1)}, \mu_h^{(n)}, \alpha_h^{(n-1)}, \alpha_h^{(n)} \in \mathrm{Lip}(\Omega)$ find $u_h^{(n+1)}, v_h^{(n+1)} \in S^h$ satisfying

$$\begin{aligned}
&\frac{1}{2\Delta t}\left(3u_h^{(n+1)} - 4u_h^{(n)} + u_h^{(n-1)}, \chi_h\right)^h + D_u\left(\nabla u_h^{(n+1)}, \nabla \chi_h\right) \\
&= \left(\frac{2r|u_h^{(n)}|^2}{|v_h^{(n)}| + \varepsilon|u_h^{(n)}|^2 + \varepsilon} - \frac{r|u_h^{(n-1)}|^2}{|v_h^{(n-1)}| + \varepsilon|u_h^{(n-1)}|^2 + \varepsilon}\right. \\
&\left. - 2\mu_h^{(n)} u_h^{(n)} + \mu_h^{(n-1)} u_h^{(n-1)} + r, \chi_h\right)^h, \\
&\frac{1}{2\Delta t}\left(3v_h^{(n+1)} - 4v_h^{(n)} + v_h^{(n-1)}, \chi_h\right)^h + D_v\left(\nabla v_h^{(n+1)}, \nabla \chi_h\right) \\
&= \left(\frac{2r|u_h^{(n)}|^2}{1 + \varepsilon|u_h^{(n)}|^2} - \frac{r|u_h^{(n-1)}|^2}{1 + \varepsilon|u_h^{(n-1)}|^2} - 2\alpha_h^{(n)} v_h^{(n)} + \alpha_h^{(n-1)} v_h^{(n-1)}, \chi_h\right)^h,
\end{aligned} \tag{7.4}$$

for all $\chi_h \in S^h$, $n = 1, 2, \dots, N$, with initial densities $u_h^{(0)} = \pi^h u_0(x)$, $v_h^{(0)} = \pi^h v_0(x)$.

The discrete cost functional used in the optimal control problem is given by

$$
\begin{aligned}
J^N = {} & \frac{\Delta t}{2}\sum_{n=1}^{N}\left(\beta_1\|u_h^{(n)}-\overline{u}_h^{(n)}\|_0^2+\beta_2\|v_h^{(n)}\overline{v}_h^{(n)}\|_0^2\right) \\
& + \frac{1}{2}\left(\gamma_1\|u_h^{(N)}-\overline{u}_h^{(N)}\|_0^2+\gamma_2\|v_h^{(N)}-\overline{v}_h^{(N)}\|_0^2\right) \\
& + \frac{\delta_1\cdot\Delta t}{2}\sum_{n=1}^{N}\|\mu_h^{(n)}\|_0^2+\frac{\delta_2\cdot\Delta t}{2}\sum_{n=1}^{N}\|\alpha_h^{(n)}\|_0^2.
\end{aligned}
\tag{7.5}
$$

Thus we can formulate the fully discrete optimal control problem as:

($\mathbf{P}^{h,\Delta t}$) Given $\Delta t = T/N$, $h = L/J$, $u_0, v_0 \in H^1(\Omega)\cap L^\infty(\Omega)$ and $\bar{u},\bar{v}\in L^2(Q)$, find $(u_h^{(n)}, v_h^{(n)}, \mu_h^{(n)}, \alpha_h^{(n)}) \in S^h\times S^h\times S^h\times S^h$ such that (7.3)-(7.4) is satisfied for $n = 1, 2, \ldots, N$ and the cost functional (7.5) is minimized.

To complete the fully discrete optimality system we also need the following fully discrete adjoint system: The adjoint functions $p_h^{(n)}, q_h^{(n)} \in S^h$ satisfy for the first time step

$$
\begin{aligned}
& \frac{1}{2\Delta t}\left(2p_h^{(0)}-4p_h^{(1)}+p_h^{(2)},\chi_h\right)^h + D_u\left(\nabla p_h^{(0)},\nabla\chi_h\right) \\
& = \left(\left(r\frac{2u_h^{(1)}(|v_h^{(1)}|+\varepsilon)}{(|v_h^{(1)}|+\varepsilon|u_h^{(1)}|^2+\varepsilon)^2}-\mu_h^{(1)}\right)\cdot(2p_h^{(1)}-p_h^{(2)}),\chi_h\right)^h \\
& + \left(\frac{2ru_h^{(1)}}{1+\varepsilon|u_h^{(1)}|^2}\cdot(2q_h^{(1)}-q_h^{(2)})+\beta_1(u_h^{(1)}-\overline{u}_h^{(1)}),\chi_h\right)^h, \\
& \frac{1}{2\Delta t}\left(2q_h^{(0)}-4q_h^{(1)}+q_h^{(2)},\chi_h\right)^h + D_v\left(\nabla q_h^{(0)},\nabla\chi_h\right) \\
& = \left(r\frac{|u_h^{(1)}|^2\mathrm{sign}(v_h^{(1)})}{(|v_h^{(1)}|+\varepsilon|u_h^{(1)}|^2+\varepsilon)^2}\cdot(-2p_h^{(1)}+p_h^{(2)}),\chi_h\right)^h \\
& + \left(\alpha_h^{(1)}(-2q_h^{(1)}+q_h^{(2)})+\beta_2(v_h^{(1)}-\overline{v}_h^{(1)}),\chi_h\right)^h,
\end{aligned}
\tag{7.6}
$$

and for $n = 2, \ldots, N-2$ we have

$$
\begin{aligned}
& \frac{1}{2\Delta t}\left(3p_h^{(n-1)}-4p_h^{(n)}+p_h^{(n+1)},\chi_h\right)^h + D_u\left(\nabla p_h^{(n-1)},\nabla\chi_h\right) \\
& = \left(\left(r\frac{2u_h^{(n)}(|v_h^{(n)}|+\varepsilon)}{(|v_h^{(n)}|+\varepsilon|u_h^{(n)}|^2+\varepsilon)^2}-\mu_h^{(n)}\right)\cdot(2p_h^{(n)}-p_h^{(n+1)}),\chi_h\right)^h \\
& + \left(\frac{2ru_h^{(n)}}{1+\varepsilon|u_h^{(n)}|^2}\cdot(2q_h^{(n)}-q_h^{(n+1)})+\beta_1(u_h^{(n)}-\overline{u}_h^{(n)}),\chi_h\right)^h,
\end{aligned}
\tag{7.7}
$$

$$\frac{1}{2\Delta t}\left(3q_h^{(n-1)}-4q_h^{(n)}+q_h^{(n+1)},\chi_h\right)^h+D_v\left(\nabla q_h^{(n-1)},\nabla\chi_h\right)$$
$$=\left(r\frac{|u_h^{(n)}|^2\mathrm{sign}(v_h^{(n)})}{(|v_h^{(n)}|+\varepsilon|u_h^{(n)}|^2+\varepsilon)^2}\cdot(-2p_h^{(n)}+p_h^{(n+1)}),\chi_h\right)^h$$
$$+\left(\alpha_h^{(n)}(-2q_h^{(n)}+q_h^{(n+1)})+\beta_2(v_h^{(n)}-\overline{v}_h^{(n)}),\chi_h\right)^h,$$

and for $n=N-1$ we have

$$\begin{aligned}(7.8)\quad &\frac{1}{2\Delta t}\left(3p_h^{(N-2)}-4p_h^{(N-1)},\chi_h\right)^h+D_u\left(\nabla p_h^{(N-2)},\nabla\chi_h\right)\\
&=\left(\left(r\frac{2u_h^{(N-1)}(|v_h^{(N-1)}|+\varepsilon)}{(|v_h^{(N-1)}|+\varepsilon|u_h^{(N-1)}|^2+\varepsilon)^2}-\mu_h^{(N-1)}\right)\cdot(2p_h^{(N-1)}-2p_h^{(N)}),\chi_h\right)^h\\
&+\left(\frac{2ru_h^{(N-1)}}{1+\varepsilon|u_h^{(N-1)}|^2}\cdot(2q_h^{(N-1)}-q_h^{(N)})+\beta_1(u_h^{(N-1)}-\overline{u}_h^{(N-1)}),\chi_h\right)^h,\\
&\frac{1}{2\Delta t}\left(3q_h^{(N-2)}-4q_h^{(N-1)},\chi_h\right)^h+D_v\left(\nabla q_h^{(N-2)},\nabla\chi_h\right)\\
&=\left(r\frac{|u_h^{(N-1)}|^2\mathrm{sign}(v_h^{(N-1)})}{(|v_h^{(N-1)}|+\varepsilon|u_h^{(N-1)}|^2+\varepsilon)^2}\cdot(-2p_h^{(N-1)}+p_h^{(N)}),\chi_h\right)^h\\
&+\left(\alpha_h^{(N-1)}(-2q_h^{(N-1)}+q_h^{(N)})+\beta_2(v_h^{(N-1)}-\overline{v}_h^{(N-1)}),\chi_h\right)^h,\end{aligned}$$

and for $n=N$ we have

$$\begin{aligned}(7.9)\quad &\frac{1}{2\Delta t}\left(3p_h^{(N-1)}-2p_h^{(N)},\chi_h\right)^h+D_u\left(\nabla p_h^{(N-1)},\nabla\chi_h\right)=\beta_1\left(u_h^{(N)}-\overline{u}_h^{(N)}),\chi_h\right)^h,\\
&\frac{1}{2\Delta t}\left(3q_h^{(N-1)}-2q_h^{(N)},\chi_h\right)^h+D_v\left(\nabla q_h^{(N-1)},\nabla\chi_h\right)=\beta_2\left(v_h^{(N)}-\overline{v}_h^{(N)}),\chi_h\right)^h,\end{aligned}$$

supplemented with the final conditions:

$$(7.10)\qquad p_h^{(N)}=\gamma_1(u_h^{(N)}-\overline{u}_h^{(N)}),\quad q_h^{(N)}=\gamma_2(v_h^{(N)}-\overline{v}_h^{(N)}).$$

THEOREM 7.1. *If $\{u_h^{(n)},v_h^{(n)}\}_{n=0}^N$ and $\{\alpha_h^{(n)},\mu_h^{(n)}\}_{n=0}^N$ are optimal for the problem (7.3)-(7.4), (7.5), then there exist $\{p_h^{(n)},q_h^{(n)}\}_{n=0}^N$ satisfying (7.6)-(7.10) such that, for $n=1,\dots,N-2$:*

$$\alpha_h^{(n)}=\frac{v_h^{(n)}}{\delta_2}(2q_h^{(n)}-q_h^{(n+1)}),\mu_h^{(n)}=\frac{u_h^{(n)}}{\delta_1}(2p_h^{(n)}-p_h^{(n+1)}),$$

for $n=N-1$:

$$\alpha_h^{(N-1)}=\frac{2v_h^{(N-1)}q_h^{(N-1)}}{\delta_2},\mu_h^{(N-1)}=\frac{2u_h^{(N-1)}p_h^{(N-1)}}{\delta_1},$$

and for $n=N$: $\qquad \alpha_h^{(N)}=\mu_h^{(N)}=0.$

For a proof see [16], which covers the numerical analysis of the work presented in this paper.

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