SpezialForschungsBereich F 32

Karl–Franzens Universität Graz
Technische Universität Graz
Medizinische Universität Graz

Optimal control of the bidomain system (III): Existence of minimizers and first-order optimality conditions

Karl Kunisch Marcus Wagner

SFB-Report No. 2011–031 December 2011

A–8010 GRAZ, HEINRICHSTRASSE 36, AUSTRIA

Supported by the
Austrian Science Fund (FWF)

SFB sponsors:

- **Austrian Science Fund** (FWF)
- **University of Graz**
- **Graz University of Technology**
- **Medical University of Graz**
- **Government of Styria**
- **City of Graz**

Das Land Steiermark

Stadt GRAZ Wissenschaft

Optimal control of the bidomain system (III): Existence of minimizers and first-order optimality conditions

Karl Kunisch and Marcus Wagner

1. Introduction.

In this work, we continue our investigations of optimal control problems for the bidomain system. After the study of the monodomain approximation of the equations and a thorough stability and regularity analysis of weak solutions for the full bidomain equations, as contained in the previous papers [Kunisch/Wagner 11a] and [Kunisch/Wagner 11b] , we are now in position to analyze the related control problems with respect to the existence of minimizers as well as to provide a rigorous proof of the first-order necessary optimality conditions.
Let $\Omega \subset \mathbb{R}^3$ be a bounded domain and $T > 0$ a fixed time horizon. Then the bidomain system, representing a well-accepted description of the electrical activity of the heart, is given by [01]

$$\frac{\partial \Phi_{tr}}{\partial t} + I_{ion}(\Phi_{tr}, W) - \operatorname{div}\big(M_i \nabla \Phi_i \big) = I_i \quad \text{for almost all } (x,t) \in \Omega \times [\,0\,,\,T\,]; \tag{1.1}$$

$$\frac{\partial \Phi_{tr}}{\partial t} + I_{ion}(\Phi_{tr}, W) + \operatorname{div}\big(M_e \nabla \Phi_e \big) = -I_e \quad \text{for almost all } (x,t) \in \Omega \times [\,0\,,\,T\,]; \tag{1.2}$$

$$\frac{\partial W}{\partial t} + G(\Phi_{tr}, W) = 0 \quad \text{for almost all } (x,t) \in \Omega \times [\,0\,,\,T\,]; \tag{1.3}$$

$$\mathfrak{n}^{\mathrm{T}} M_i \nabla \Phi_i = 0 \quad \text{for all } (x,t) \in \partial\Omega \times [\,0\,,\,T\,]; \tag{1.4}$$

$$\mathfrak{n}^{\mathrm{T}} M_e \nabla \Phi_e = 0 \quad \text{for all } (x,t) \in \partial\Omega \times [\,0\,,\,T\,]; \tag{1.5}$$

$$\Phi_{tr}(x,0) = \Phi_i(x,0) - \Phi_e(x,0) = \Phi_0(x) \quad \text{and} \quad W(x,0) = W_0(x) \quad \text{for almost all } x \in \Omega\,. \tag{1.6}$$

In this model, Ω represents the spatial domain occupied by the cardiac muscle, the variables Φ_i and Φ_e denote the intracellular and extracellular electric potentials, and $\Phi_{tr} = \Phi_i - \Phi_e$ is the transmembrane potential. The anisotropic electric properties of the intracellular and the extracellular tissue parts are modeled by conductivity tensors M_i and M_e. The specification of the model for the ionic current I_{ion} in (1.1) and (1.2) and the gating function G in (1.3) will be made below. We shall consider three so-called two-variable models wherein I_{ion} and G depend on Φ_{tr} as well as on a single gating variable W, which describes in a cumulative way the effects of the ion transport through the cell membranes (see Subsection 2.b)). Finally, the inhomogeneities I_i and I_e represent the intracellular and extracellular stimulation currents, respectively. We shall investigate optimal control problems of the form

$$\text{(P)} \quad F(\Phi_{tr}, \Phi_e, W, I_e) = \int_0^T \!\! \int_\Omega r\big(x, t, \Phi_{tr}(x,t), \Phi_e(x,t), W(x,t) \big)\, dx\, dt + \frac{\mu}{2} \int_0^T \!\! \int_{\Omega_{con}} I_e(x,t)^2\, dx\, dt \longrightarrow \inf! \tag{1.7}$$

subject to the bidomain equations (1.1) – (1.6) in its weak formulation (see (2.1) – (2.4) below)

and the control restriction $I_e \in \mathcal{C}$ (1.8)

---

[01] The bidomain model has been considered first in [Tung 78] . A detailed introduction may be found e. g. in [Sundnes/ Lines/Cai/Nielsen/Mardal/Tveito 06] , pp. 21 – 56.

where

$$\mathcal{C} \,=\, \big\{\, Q\,I \;\big|\; I \in L^\infty\big[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\,\big]\,,\ \operatorname{supp}(I) \subseteq \Omega_{con} \times [\,0\,,\,T\,]\,, \qquad (1.9)$$
$$|\,I(x,t)\,| \,\leqslant\, R \ \ (\forall)\,(x,t) \in \Omega_T \,\big\} \,\subset\, L^\infty\big[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\,\big]\,.$$

For the description of the control domain, the linear operator $Q\colon\ L^2(\Omega_T) \to L^2(\Omega_T)$ defined by

$$Q\,I(x,t) \,=\, I(x,t) - \mathbb{1}_{\Omega_{con}}(x) \cdot \frac{1}{|\,\Omega_{con}\,|} \int_{\Omega_{con}} I(\tilde{x},t)\,d\tilde{x} \qquad (1.10)$$

has been used. When applied to a function I with $\operatorname{supp}(I) \subseteq \Omega_{con} \times [\,0\,,\,T\,]$, Q extends by zero the orthogonal projection onto the complement of the subspace $\{\,Z \;\big|\; \int_{\Omega_{con}} Z(\tilde{x},t)\,d\tilde{x} = 0$ for a. a. $t \in (\,0\,,\,T\,)\,\} \subset L^2\big[\,(\,0\,,\,T\,)\,,\,L^2(\Omega_{con})\,\big]$. Consequently, for $I_e \in \mathcal{C}$, we have

$$\int_\Omega I_e(x,t)\,dx \,=\, \int_{\Omega_{con}} I_e(x,t)\,dx \,=\, 0 \quad \text{for almost all } t \in (\,0\,,\,T\,)\,, \qquad (1.11)$$

what guarantees the solvability of the state equations (cf. Theorem 2.3. below). In problem (P), the extracellular excitation I_e acts as control, which is allowed to be applied on the subdomain Ω_{con} only.[02] The pointwise constraint within the description (1.9) of $\mathcal{C}$ is included due to the obvious fact that one cannot apply arbitrary large electrical stimulations to living tissue without damaging it. In mathematical terms, this restriction is necessary in order to establish a stability estimate for the bidomain system (Theorem 2.4.).
For the first term within the objective (1.7), a typical choice is a tracking-type integrand related to a desired state of the system. The integrand $r(x,t,\varphi,\eta,w)$ should be measurable w. r. to x and t and smooth w. r. to the other variables. The second term expresses the requirement that — regardless of whether the pointwise restriction within (1.9) is active — the overall stimulus should be as small as possible. Consequently, solutions with little intervention to the cardiac system are favored.
Besides an existence theorem for global minimizers (Theorem 3.4.), the main result of the present paper is the rigorous proof of the following *set of first-order necessary optimality conditions* for weak local minimizers $(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e\,)$ of (P), consisting of the variational inequality

$$\int_0^T \int_{\Omega_{con}} \Big(\mu\,\hat{I}_e - Q\,P_2\Big) \cdot \big(\,I_e - \hat{I}_e\,\big)\,dx\,dt \,\geqslant\, 0 \quad \text{for all admissible controls } I_e \qquad (1.12)$$

and the adjoint system

$$\int_0^T \int_\Omega \Big(-\frac{\partial P_1}{\partial t} + \frac{\partial I_{ion}}{\partial \varphi}(\hat{\Phi}_{tr}, \hat{W})\,P_1 + \frac{\partial G}{\partial \varphi}(\hat{\Phi}_{tr}, \hat{W})\,P_3\Big)\,\psi\,dx\,dt \,+\, \int_0^T \int_\Omega \nabla\psi^{\mathrm{T}}\,M_i\,\big(\,\nabla P_1 + \nabla P_2\,\big)\,dx\,dt \quad (1.13)$$
$$= -\int_0^T \int_\Omega \Big(\,\frac{\partial r}{\partial \varphi}(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W})\Big)\,\psi\,dx\,dt \quad \forall\,\psi \in L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big]\,,\ P_1(x,T) \equiv 0\,;$$

$$\int_0^T \int_\Omega \nabla\psi^{\mathrm{T}}\,M_i\,\nabla P_1\,dx\,dt \,+\, \int_0^T \int_\Omega \nabla\psi^{\mathrm{T}}\,(M_i + M_e)\,\nabla P_2\,dx\,dt \,=\, -\int_0^T \int_\Omega \frac{\partial r}{\partial \eta}(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W})\,\psi\,dx\,dt \qquad (1.14)$$
$$\forall\,\psi \in L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big] \text{ with } \int_\Omega \psi(x,t)\,dx = 0 \text{ for a. a. } t \in (\,0\,,\,T\,)\,,\ \int_\Omega P_2(x,t)\,dx = 0\ (\forall)\,t \in (\,0\,,\,T\,)\,;$$

$$\int_0^T \int_\Omega \Big(-\frac{\partial P_3}{\partial t} + \frac{\partial I_{ion}}{\partial w}(\hat{\Phi}_{tr}, \hat{W})\,P_1 + \frac{\partial G}{\partial w}(\hat{\Phi}_{tr}, \hat{W})\,P_3\Big)\,\psi\,dx\,dt \,=\, -\int_0^T \int_\Omega \Big(\,\frac{\partial r}{\partial w}(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W})\Big)\,\psi\,dx\,dt \quad (1.15)$$
$$\forall\,\psi \in L^2\big[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\,\big]\,,\ P_3(x,T) \equiv 0$$

---

[02] For physiological reasons, the intracellular excitation I_i must be set zero.

for the multipliers P_1, P_2 and P_3 related to the weak state equations (2.1), (2.2) and (2.3) below, respectively (Theorem 5.2.). The proof, which will be given by fitting the problem (P) into the framework of *weakly singular problems* in the sense of ITO/KUNISCH, [03] is based on two main ingredients. The first one is a stability estimate for the primal equations (Theorem 2.4.), whose proof has been already provided in the previous publication [KUNISCH/WAGNER 11B] . Secondly, we need an existence proof for weak solutions of the adjoint system, which is contained in the present paper (Theorem 4.2.).

In the literature, only a few studies related to the optimal control of the bidomain system are available as yet, mostly restricted to the monodomain approximation. We mention [AINSEBA/BENDAHMANE/RUIZ-BAIER 10] , [BRANDÃO/FERNÁNDEZ-CARA/MAGALHÃES/ROJAS-MEDAR 08] , [MUZDEKA/BARBIERI 05] , [KUNISCH/NAGAIAH/WAGNER 11] , [NAGAIAH/KUNISCH 11] and [NAGAIAH/KUNISCH/PLANK 11] and refer to [KUNISCH/WAGNER 11A] , p. 3, for a closer discussion.

The paper is structured in the following way. In Section 2, the weak solution concept for the bidomain equations is outlined. We present the ionic models to be used and summarize the existence and stability theorems for weak solutions of (1.1) – (1.6). Then, in Section 3, we restate the optimal control problem (1.7) – (1.8) within function spaces, subsequently analyzing the structure of the feasible domain and establishing the existence of global minimizers. Section 4 is concerned with the derivation of the adjoint system and the existence proof for a weak solution of it. Finally, in Section 5, we state and prove the first-order necessary optimality conditions for the control problem.

Notations.

We denote by $L^p(\Omega)$ the space of functions, which are in the pth power integrable ($1 \leqslant p < \infty$), or are measurable and essentially bounded ($p = \infty$), and by $W^{1,p}(\Omega)$ the Sobolev space of functions $\psi\colon\ \Omega \to \mathbb{R}$ which, together with their first-order weak partial derivatives, belong to the space $L^p(\Omega, \mathbb{R})$ ($1 \leqslant p < \infty$). For spaces of Bochner integrable mappings, e. g. $L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big]$, we refer to the summary in [KUNISCH/WAGNER 11A] , p. 20 f. Ω_T is an abbreviation for $\Omega \times [\,0\,,\,T\,]$. The gradient ∇ is always taken only with respect to the spatial variables x. The characteristic function of the set $\mathrm{A} \subseteq \mathbb{R}^3$ is defined as $\mathbb{1}_{\mathrm{A}}\colon\ \mathbb{R}^3 \to \mathbb{R}$ with $\mathbb{1}_{\mathrm{A}}(x) = 1 \iff x \in \mathrm{A}$ and $\mathbb{1}_{\mathrm{A}}(x) = 0 \iff x \notin \mathrm{A}$. Finally, the nonstandard abbreviation "$(\forall)\, t \in \mathrm{A}$" has to be read as "for almost all $t \in \mathrm{A}$" or "for all $t \in \mathrm{A}$ except for a Lebesgue null set", and the symbol $\mathfrak{o}$ denotes, depending on the context, the zero element or the zero function of the underlying space.

2. Weak solutions of the bidomain system.

a) Parabolic-elliptic form of the bidomain system; weak solutions.

It is well-known that the bidomain system (1.1) – (1.6) can be equivalently stated in parabolic-elliptic form. [04] In its weak formulation, the system reads as follows:

$$\int_\Omega \Big(\frac{\partial \Phi_{tr}}{\partial t} \cdot \psi + \nabla\psi^{\mathrm{T}} M_i (\, \nabla\Phi_{tr} + \nabla\Phi_e\,) + I_{ion}(\Phi_{tr}, W)\, \psi \Big)\, dx \;=\; \int_\Omega I_i\, \psi\, dx \tag{2.1}$$

$$\forall\, \psi \in W^{1,2}(\Omega)\,, \ \text{ for a. a. } t \in (\,0\,,\,T\,)\,;$$

$$\int_\Omega \Big(\nabla\psi^{\mathrm{T}} M_i \nabla\Phi_{tr} + \nabla\psi^{\mathrm{T}} (M_i + M_e)\, \nabla\Phi_e \Big)\, dx \;=\; \int_\Omega \Big(I_i + I_e \Big)\, \psi\, dx \tag{2.2}$$

$$\forall\, \psi \in W^{1,2}(\Omega) \ \text{ with } \ \int_\Omega \psi(x)\, dx = 0\,, \ \text{ for a. a. } t \in (\,0\,,\,T\,)\,;$$

---

[03] [ITO/KUNISCH 08] , p. 17 f.

[04] Cf. [BOURGAULT/COUDIÈRE/PIERRE 09] , p. 459, and [KUNISCH/WAGNER 11B] , p. 4, (2.1) – (2.6)

$$\int_\Omega \Big(\frac{\partial W}{\partial t} + G(\Phi_{tr}, W) \Big)\, \psi \, dx \;=\; 0 \quad \forall\, \psi \in L^2(\Omega)\,, \;\text{ for a. a. } t \in (\,0\,,\,T\,)\,; \tag{2.3}$$

$$\Phi_{tr}(x,0) \;=\; \Phi_0(x) \quad \text{and} \quad W(x,0) \;=\; W_0(x) \quad \text{for almost all } x \in \Omega\,. \tag{2.4}$$

Throughout the paper, the following assumptions about the data will be made:

Assumptions 2.1. (Basic assumptions on the data)

1) $\Omega \subset \mathbb{R}^3$ *is a bounded Lipschitz domain.*

2) $M_i,\, M_e :\ \mathrm{cl}\,(\Omega) \to \mathbb{R}^{3\times 3}$ *are symmetric, positive definite matrix functions with* $L^\infty(\Omega)$*-coefficients, obeying uniform ellipticity conditions:*

$$0 \leqslant \mu_1 \,\|\, \xi \,\|^2 \leqslant \xi^{\mathrm{T}} M_i(x)\, \xi \leqslant \mu_2 \,\|\, \xi \,\|^2 \quad \textit{and} \quad 0 \leqslant \mu_1 \,\|\, \xi \,\|^2 \leqslant \xi^{\mathrm{T}} M_e(x)\, \xi \leqslant \mu_2 \,\|\, \xi \,\|^2 \quad \forall\, \xi \in \mathbb{R}^3 \;\; \forall\, x \in \Omega \tag{2.5}$$

with $\mu_1,\ \mu_2 > 0$.

3) The initial values Φ_0 *and* W_0 *belong to the spaces* $L^2(\Omega)$ *and* $L^4(\Omega)$*, respectively.*

The notion of a weak solution is as follows:

Definition 2.2. (Weak solution of the bidomain system) [05] *A triple* (Φ_{tr}, Φ_e, W) *is called a weak solution of the bidomain system* (2.1) − (2.4) *on* $[\,0\,,\,T\,]$ *iff the functions* Φ_{tr}, Φ_e *and* W *satisfy* (2.1) − (2.4) *and belong to the spaces*

$$\Phi_{tr} \in C^0\big[\,[\,0\,,\,T\,]\,,\,L^2(\Omega)\,\big] \,\cap\, L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big] \,\cap\, L^4(\Omega_T)\,; \tag{2.6}$$

$$\Phi_e \in L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big]\,; \tag{2.7}$$

$$W \in C^0\big[\,[\,0\,,\,T\,]\,,\,L^2(\Omega)\,\big] \tag{2.8}$$

while $\int_\Omega \Phi_e(x,t)\, dx \;=\; 0$ *holds for almost all* $t \in (\,0\,,\,T\,)$.

b) Two-variable models for the ionic current.

For the ionic current I_{ion} and the function G within the gating equation, the following three models will be considered:

a) The Rogers-McCulloch model. [06]

$$I_{ion}(\varphi, w) \;=\; b \cdot \varphi\, (\varphi - a)\, (\varphi - 1) + \varphi \cdot w \;=\; b\, \varphi^3 - (a+1)\, b\, \varphi^2 + a\, b\, \varphi + \varphi\, w\,; \tag{2.9}$$

$$G(\varphi, w) \;=\; \varepsilon\, w - \varepsilon\, \kappa\, \varphi \tag{2.10}$$

with $0 < a < 1$, $b > 0$, $\kappa > 0$ and $\varepsilon > 0$. Consequently, the gating variable obeys the linear ODE

$$\partial W/\partial t + \varepsilon\, W \;=\; \varepsilon\, \kappa\, \Phi_{tr}\,. \tag{2.11}$$

b) The FitzHugh-Nagumo model. [07]

$$I_{ion}(\varphi, w) \;=\; \varphi\, (\varphi - a)\, (\varphi - 1) + w \;=\; \varphi^3 - (a+1)\, \varphi^2 + a\, \varphi + w\,; \tag{2.12}$$

$$G(\varphi, w) \;=\; \varepsilon\, w - \varepsilon\, \kappa\, \varphi \tag{2.13}$$

---

[05] [Bourgault/Coudière/Pierre 09] , p. 472, Definition 26.

[06] [Rogers/McCulloch 94] .

[07] [FitzHugh 61] , together with [Nagumo/Arimoto/Yoshizawa 62] .

with $0 < a < 1$, $\kappa > 0$ and $\varepsilon > 0$. Consequently, the gating variable obeys the same linear ODE (2.11) as before.

c) The linearized Aliev-Panfilov model. [08)]

$$I_{ion}(\varphi, w) = b \cdot \varphi\,(\varphi - a)\,(\varphi - 1) + \varphi \cdot w = b\,\varphi^3 - (a+1)\,b\,\varphi^2 + a\,b\,\varphi + \varphi\,w\,; \tag{2.14}$$

$$G(\varphi, w) = \varepsilon\,w - \varepsilon\,\kappa\,\big(\,(a+1)\,\varphi - \varphi^2\,\big) \tag{2.15}$$

with $0 < a < 1$, $b > 0$, $\kappa > 0$ and $\varepsilon > 0$. The linear ODE for the gating variable is

$$\partial W/\partial t + \varepsilon\,W = \varepsilon\,\kappa\,\big(\,(a+1)\,\Phi_{tr} - {\Phi_{tr}}^2\,\big)\,. \tag{2.16}$$

c) Existence and uniqueness of weak solutions; the stability estimate.

In [Kunisch/Wagner 11b] , the following results about weak solutions of the bidomain system (2.1) – (2.4) have been obtained:

Theorem 2.3. (Existence and uniqueness of weak solutions) [09)] *Assume that the data within* (2.1) – (2.4) *obey Assumptions 2.1., and specify any of the three models described in Subsection 2.b). Then the bidomain system* (2.1) – (2.4) *admits for arbitrary initial values* $\Phi_0 \in L^2(\Omega)$, $W_0 \in L^4(\Omega)$ *and inhomogeneities* $I_i,\ I_e \in L^\infty\big[\,(\,0\,,\,T\,)\,,\,\big(\,W^{1,2}(\Omega)\,\big)^*\,\big]$, *which satisfy the compatibility condition*

$$\int_\Omega \Big(\,I_i(x,t) + I_e(x,t)\,\Big)\,dx = 0 \quad \textit{for almost all } t \in (\,0\,,\,T\,)\,, \tag{2.17}$$

a uniquely determined weak solution (Φ_{tr}, Φ_e, W) *on* $[\,0\,,\,T\,]$ *according to Definition 2.2.*

Theorem 2.4. (Stability estimate for weak solutions) [10)] *Assume that the data within* (2.1) – (2.4) *obey Assumptions 2.1., and specify any of the three models described in Subsection 2.b). Consider two weak solutions* $({\Phi_{tr}}', {\Phi_e}', W')$, $({\Phi_{tr}}'', {\Phi_e}'', W'')$ *of* (2.1) – (2.4), *which correspond to initial values* $\Phi_0' = \Phi_0'' = \Phi_0 \in L^2(\Omega)$, $W_0' = W_0'' = W_0 \in L^4(\Omega)$ *and inhomogeneities* ${I_i}'$, ${I_e}'$, ${I_i}''$ *and* ${I_e}'' \in L^\infty\big[\,(\,0\,,\,T\,)\,,\,\big(\,W^{1,2}(\Omega)\,\big)^*\,\big]$ *with*

$$\int_\Omega \Big(\,{I_i}'(x,t) + {I_e}'(x,t)\,\Big)\,dx = \int_\Omega \Big(\,{I_i}''(x,t) + {I_e}''(x,t)\,\Big)\,dx = 0 \quad \textit{for almost all } t \in (\,0\,,\,T\,)\,, \tag{2.18}$$

whose norms are bounded by $R > 0$. *Then the following estimates hold:*

$$\begin{aligned} &\|\,{\Phi_{tr}}' - {\Phi_{tr}}''\,\|^2_{L^2[\,(0,T),\,W^{1,2}(\Omega)\,]} + \|\,{\Phi_{tr}}' - {\Phi_{tr}}''\,\|^2_{C^0[\,[0,T],\,L^2(\Omega)\,]} + \|\,{\Phi_e}' - {\Phi_e}''\,\|^2_{L^2[\,(0,T),\,W^{1,2}(\Omega)\,]} \\ &\quad + \|\,W' - W''\,\|^2_{L^2[\,(0,T),\,L^2(\Omega)\,]} + \|\,W' - W''\,\|^2_{C^0[\,[0,T],\,L^2(\Omega)\,]} + \|\,W' - W''\,\|^2_{W^{1,2}[\,(0,T),\,L^2(\Omega)\,]} \\ &\qquad \leqslant C\,\Big(\,\|\,{I_i}' - {I_i}''\,\|^2_{L^\infty[\,(0,T),\,(W^{1,2}(\Omega))^*\,]} + \|\,{I_e}' - {I_e}''\,\|^2_{L^\infty[\,(0,T),\,(W^{1,2}(\Omega))^*\,]}\,\Big)\,; \end{aligned} \tag{2.19}$$

$$\begin{aligned} &\|\,{\Phi_{tr}}' - {\Phi_{tr}}''\,\|_{W^{1,4/3}[\,(0,T),\,(W^{1,2}(\Omega))^*\,]} \leqslant C \cdot \mathrm{Max}\,\Big(\,\|\,{I_i}' - {I_i}''\,\|_{L^2[\,(0,T),\,(W^{1,2}(\Omega))^*\,]}\,, \\ &\|\,{I_e}' - {I_e}''\,\|_{L^2[\,(0,T),\,(W^{1,2}(\Omega))^*\,]}\,,\,\|\,{I_i}' - {I_i}''\,\|^2_{L^2[\,(0,T),\,(W^{1,2}(\Omega))^*\,]}\,,\,\|\,{I_e}' - {I_e}''\,\|^2_{L^2[\,(0,T),\,(W^{1,2}(\Omega))^*\,]}\,\Big)\,. \end{aligned} \tag{2.20}$$

---

08) See [Aliev/Panfilov 96] . The linearized model is taken from [Bourgault/Coudière/Pierre 09] , p. 480.

09) [Bourgault/Coudière/Pierre 09] , p. 473, Theorem 30, together with [Kunisch/Wagner 11b] , p. 8, Theorem 2.8.

10) [Kunisch/Wagner 11b] , p. 7 f., Theorem 2.7.

The constant $C > 0$ does not depend on I_i', I_e', I_i'' and I_e'' but possibly on Ω, R, Φ_0 and W_0.

The assumptions in Theorems 2.2. and 2.3. are in accordance to the analytical framework wherein the control problem (P) will be studied in the next sections.

3. The optimal control problem.

a) Formulation of the problem within function spaces.

In order to provide a precise statement of the optimal control problem (P) (1.7) − (1.8) within an appropriate function space framework, we introduce the following spaces:

$$\mathrm{X}_1 \,=\, L^2\big[\,(\,0\,,T\,)\,,\,W^{1,2}(\Omega)\,\big]\,;\quad \mathrm{X}_2 \,=\, \mathrm{X}_1 \cap \big\{\,Z \;\big|\; \int_\Omega Z(x,t)\,dx = 0\ \ (\forall)\,t \in (\,0\,,T\,)\,\big\}\,; \tag{3.1}$$

$$\mathrm{X}_3 \,=\, L^2\big[\,(\,0\,,T\,)\,,\,L^2(\Omega)\,\big]\,;\quad \mathrm{X}_4 \,=\, L^\infty\big[\,(\,0\,,T\,)\,,\,L^2(\Omega)\,\big]\,. \tag{3.2}$$

We will further specify the subspaces

$$\widetilde{\mathrm{X}}_1 \,=\, \mathrm{X}_1 \cap W^{1,4/3}\big[\,(\,0\,,T\,)\,,\,\big(W^{1,2}(\Omega)\big)^*\,\big] \cap C^0\big[\,[\,0\,,T\,]\,,\,L^2(\Omega)\,\big]\,;\quad \widetilde{\mathrm{X}}_2 \,=\, \mathrm{X}_2\,; \tag{3.3}$$

$$\widetilde{\mathrm{X}}_3 \,=\, \mathrm{X}_3 \cap W^{1,2}\big[\,(\,0\,,T\,)\,,\,\big(L^2(\Omega)\big)^*\,\big] \cap C^0\big[\,[\,0\,,T\,]\,,\,L^2(\Omega)\,\big]\,, \tag{3.4}$$

which contain all polynomials and, consequently, lie dense in X_1, X_2 and X_3, as well as the target spaces

$$\mathrm{Z}_1 \,=\, L^{4/3}\big[\,(\,0\,,T\,)\,,\,\big(W^{1,2}(\Omega)\big)^*\,\big]\,;\quad \mathrm{Z}_2 \,=\, L^2\big[\,(\,0\,,T\,)\,,\,\big(W^{1,2}(\Omega)\big)^*\,\big]\,; \tag{3.5}$$

$$\mathrm{Z}_3 \,=\, L^2\big[\,(\,0\,,T\,)\,,\,\big(L^2(\Omega)\big)^*\,\big]\,;\quad \mathrm{Z}_4 \,=\, Z_5 \,=\, L^2(\Omega)\,. \tag{3.6}$$

The quadruples $(\Phi_{tr}, \Phi_e, W, I_e)$ of state and control variables will be chosen from the space $\widetilde{\mathrm{X}}_1 \times \widetilde{\mathrm{X}}_2 \times \widetilde{\mathrm{X}}_3 \times \mathrm{X}_4$. Recall the definition of $Q\colon\, L^2(\Omega_T) \to L^2(\Omega_T)$ as

$$Q\,I(x,t) \,=\, I(x,t) - \mathbb{1}_{\Omega_{con}}(x) \cdot \frac{1}{|\,\Omega_{con}\,|} \int_{\Omega_{con}} I(\tilde{x},t)\,d\tilde{x}\,. \tag{3.7}$$

With the aid of the operators

$$F\colon\, \mathrm{X}_1 \times \mathrm{X}_2 \times \mathrm{X}_3 \times \mathrm{X}_4 \to \mathbb{R}\,; \tag{3.8}$$

$$E_1\colon\, \widetilde{\mathrm{X}}_1 \times \widetilde{\mathrm{X}}_2 \times \widetilde{\mathrm{X}}_3 \to \mathrm{Z}_1\,;\quad E_2\colon\, \widetilde{\mathrm{X}}_1 \times \widetilde{\mathrm{X}}_2 \times \mathrm{X}_4 \to \mathrm{Z}_2\,;\quad E_3\colon\, \widetilde{\mathrm{X}}_1 \times \widetilde{\mathrm{X}}_3 \to \mathrm{Z}_3\,; \tag{3.9}$$

$$E_4\colon\, \widetilde{\mathrm{X}}_1 \to \mathrm{Z}_4\,;\quad E_5\colon\, \widetilde{\mathrm{X}}_3 \to \mathrm{Z}_5\,, \tag{3.10}$$

the problem (P) will be restated now in the following way:

$$(\mathrm{P})\quad F(\Phi_{tr}, \Phi_e, W, I_e) \,=\, \int_0^T \int_\Omega r\big(\,x, t, \Phi_{tr}(x,t), \Phi_e(x,t), W(x,t)\,\big)\,dx\,dt \tag{3.11}$$

$$+\, \frac{\mu}{2} \cdot \int_0^T \int_\Omega I_e(x,t)^2\,dx\,dt \longrightarrow \inf!\,;$$

$$E_1(\Phi_{tr}, \Phi_e, W) \,=\, \int_\Omega \Big(\,\frac{\partial \Phi_{tr}}{\partial t} + I_{ion}(\Phi_{tr}, W)\,\Big)\,\psi\,dx + \int_\Omega \nabla\psi^{\mathrm{T}} M_i (\,\nabla\Phi_{tr} + \nabla\Phi_e\,)\,dx \,=\, 0 \tag{3.12}$$

$$\forall\,\psi \in W^{1,2}(\Omega)\ \ (\forall)\,t \in (\,0\,,T\,)\,;$$

$$E_2(\Phi_{tr}, \Phi_e, I_e) \,=\, \int_\Omega \Big(\,\nabla\psi^{\mathrm{T}} M_i \nabla\Phi_{tr} + \nabla\psi^{\mathrm{T}}(M_i + M_e)\,\nabla\Phi_e\,\Big)\,dx - \int_\Omega I_e\,\psi\,dx \,=\, 0 \tag{3.13}$$

$$\forall\,\psi \in W^{1,2}(\Omega)\ \text{ with }\ \int_\Omega \psi(x)\,dx = 0\ \ (\forall)\,t \in (\,0\,,T\,)\,;$$

$$E_3(\Phi_{tr}, W) \,=\, \int_\Omega \Big(\,\frac{\partial W(t)}{\partial t} + G(\Phi_{tr}(t), W(t))\,\Big)\,\psi\,dx \,=\, 0 \quad \forall\,\psi \in L^2(\Omega)\ \ (\forall)\,t \in (\,0\,,T\,)\,; \tag{3.14}$$

$$E_4(\Phi_{tr}) \;=\; \Phi_{tr}(x,0) - \Phi_0(x) \;=\; 0 \quad (\forall)\, x \in \Omega\,; \tag{3.15}$$

$$E_5(W) \;=\; W(x,0) - W_0(x) \;=\; 0 \quad (\forall)\, x \in \Omega\,; \tag{3.16}$$

$$I_e \in \mathcal{C} \;=\; \big\{\, Q\, I \;\big|\; I \in L^\infty\big[\,(\,0\,,\,T\,)\,,\, L^2(\Omega)\,\big]\,,\ \mathrm{supp}\,(I) \subseteq \Omega_{con} \times [\,0\,,\,T\,]\,, \quad | \, I(x,t)\, | \,\leqslant\, R\;\; (\forall)\,(x,t) \in \Omega_T \,\big\} \,\subset\, L^\infty\big[\,(\,0\,,\,T\,)\,,\, L^2(\Omega)\,\big]\,. \tag{3.17}$$

Assumptions 2.1. are imposed on the data of problem (P). The numbers $T > 0$, $\mu > 0$ and $R > 0$, the functions $\Phi_0 \in L^2(\Omega)$ and $W_0 \in L^4(\Omega)$ as well as the Lipschitz subdomain $\Omega_{con} \subseteq \Omega$ are fixed. The functions I_{ion} and G will be specified according to any of the models from Subsection 2.b). Concerning the objective functional F, we assume the integrand

$$r(x,t,\varphi,\eta,w)\colon\; \Omega \,\times\, [\,0\,,\,T\,] \,\times\, \mathbb{R}^3 \to \mathbb{R} \tag{3.18}$$

to be measurable with respect to x and t and continuous with respect to φ, η and w. With regard to (3.7) and (3.17), in the second term of F the original integration domain Ω_{con} from (1.7) can be replaced by Ω.

b) Structure of the feasible domain.

Proposition 3.1. *The control-to-state-mapping* $\mathcal{C} \ni I_e \longmapsto (\Phi_{tr}, \Phi_e, W) \in \mathrm{X}_1 \,\times\, \mathrm{X}_2 \,\times\, \mathrm{X}_3$ *is well-defined.*

Proof. Recall that $\int_\Omega I_e(x,t)\, dx = 0$ for almost all $t \in (\,0\,,\,T\,)$. Consequently, the data within the problem (3.11) – (3.17) satisfy the assumptions of Theorem 2.3. with $I_i = \mathfrak{o}$, and the existence of a uniquely determined weak solution (Φ_{tr}, Φ_e, W) of the bidomain system is guaranteed for any feasible control $I_e \in \mathcal{C} \subset L^\infty\big[\,(\,0\,,\,T\,)\,,\, L^2(\Omega)\,\big]$. ∎

Proposition 3.2. *The control domain* $\mathcal{C} \subset L^\infty(\Omega_T)$ *forms a closed, convex, weak**-*sequentially compact subset of the space* X_4.

Proof. Obviously, $\mathcal{C}$ is a convex subset of X_4. In order to confirm closedness, consider a norm-convergent sequence $\{\, Q\, I^N \,\}$ with members in $\mathcal{C} \cap \mathrm{X}_4$ and limit element $\hat{I}$. Since the sequence $\{\, I^N \,\}$ of the generating functions is uniformly bounded in $L^\infty\big[\,(\,0\,,\,T\,)\,,\, L^2(\Omega_{con})\,\big]$, it admits a weak*-convergent subsequence $I^{N'}$ with a limit element $\tilde{I}$ still satisfying the conditions $\mathrm{supp}\,(\tilde{I}) \subseteq \Omega_{con} \times [\,0\,,\,T\,]$ and $|\,\tilde{I}(x,t)\,| \leqslant R\; (\forall)\,(x,t) \in \Omega_T$. The weak*-continuity of the operator Q implies then $Q\, I^{N'} \xrightarrow{\;*\;}{}^{\mathrm{X}_4}\, Q\, \tilde{I}$ and $\hat{I} = Q\, \tilde{I} \in \mathcal{C}$. Now the weak*-sequential compactness of $\mathcal{C}$ is obtained from [Rolewicz 76] , p. 301, Theorem VI.6.6., together with p. 152, Theorem IV.4.11. Finally, $\|\, I \,\|_{L^\infty(\Omega_T)} \leqslant R$ implies $\|\, Q\, I \,\|_{L^\infty(\Omega_T)} \leqslant 2\, R$, and $\mathcal{C}$ belongs even to $L^\infty(\Omega_T)$. ∎

Proposition 3.3. *The feasible domain* $\mathcal{B}$ *of the problem* (P) *is nonempty and closed with respect to the following topology in* $\mathrm{X}_1 \times \mathrm{X}_2 \times \mathrm{X}_3 \times \mathrm{X}_4$*: weak convergence with respect to the first three components, and weak***-convergence with respect to the fourth component.*

Proof. The existence of feasible solutions follows via Theorem 2.3. from Proposition 3.1. Consider now a sequence of feasible solutions $\{\, ({\Phi_{tr}}^N, {\Phi_e}^N, W^N, {I_e}^N) \,\}$ with ${\Phi_{tr}}^N \rightharpoonup^{\mathrm{X}_1} \hat{\Phi}_{tr}$, ${\Phi_e}^N \rightharpoonup^{\mathrm{X}_2} \hat{\Phi}_e$, $W^N \rightharpoonup^{\mathrm{X}_3} \hat{W}$ and ${I_e}^N \xrightarrow{\;*\;}{}^{\mathrm{X}_4} \hat{I}_e$. From Proposition 3.2. we already know that $\hat{I}_e$ belongs to $\mathcal{C}$. Further, from [Kunisch/ Wagner 11b] , p. 7, Theorem 2.6., we obtain uniform bounds with respect to N for the norms of ${\Phi_{tr}}^N$, ${\Phi_e}^N$, W^N, $\partial{\Phi_{tr}}^N/\partial t$ and $\partial W^N/\partial t$, implying weak convergence of $\partial{\Phi_{tr}}^{N'}/\partial t$, $\nabla{\Phi_{tr}}^{N'}$ and $\partial W^{N'}/\partial t$ as well as a. e. pointwise convergence of ${\Phi_{tr}}^{N'}$ on Ω_T along a suitable subsequence. Consequently, passing to the limit $N' \to \infty$ in (2.1) – (2.4), we may confirm that $(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W})$ solves the bidomain system with right-hand sides $I_i = \mathfrak{o}$ and $\hat{I}_e$. ∎

c) Existence of global minimizers.

Theorem 3.4. (Existence of global minimizers in (P)**)** *We impose the assumptions from Subsection 3.a) on the data of* (P)*. Assume further that the integrand* $r(x,t,\varphi,\eta,w)\colon \Omega \times [\,0\,,\,T\,] \times \mathbb{R}^3 \to \mathbb{R}$ *is bounded from below and convex with respect to* φ*,* η *and* w*. Then the problem* (P) *admits a global minimizer.*

Proof. Since r is bounded from below, the problem (P) admits a minimizing sequence $\{\,({\Phi_{tr}}^N, {\Phi_e}^N, W^N, {I_e}^N)\,\}$ of feasible solutions. Due to the uniform boundedness of $\|\,{I_e}^N\,\|_{\mathrm{X}_4}$ with respect to N, the norms $\|\,{\Phi_{tr}}^N\,\|_{\mathrm{X}_1}$, $\|\,{\Phi_e}^N\,\|_{\mathrm{X}_2}$ and $\|\,W^N\,\|_{\mathrm{X}_3}$ are uniformly bounded as well (cf. again [Kunisch/Wagner 11b], p. 7, Theorem 2.6.), and we may pass to a subsequence $\{\,({\Phi_{tr}}^{N'}, {\Phi_e}^{N'}, W^{N'}, {I_e}^{N'})\,\}$, which converges to a feasible quadruple $(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ in the sense of Proposition 3.3. The lower semicontinuity of the objective follows as in [Dacorogna 08], p. 96, Theorem 3.23., and p. 97, Remark 3.25.(ii). Consequently, denoting the minimal value of (P) by m, we get

$$m \,=\, \lim_{N'\to\infty} F({\Phi_{tr}}^{N'}, {\Phi_e}^{N'}, W^{N'}, {I_e}^{N'}) \tag{3.19}$$

$$\geqslant \liminf_{N'\to\infty} F({\Phi_{tr}}^{N'}, {\Phi_e}^{N}p, W^{N'}, {I_e}^{N'}) \,\geqslant\, F(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e) \,\geqslant\, m\,,$$

and the quadruple $(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ is a global minimizer of (P). ∎

4. The adjoint equations.

a) Derivation of the adjoint system.

Throughout the following sections, we will further assume that the integrand $r(x,t,\varphi,\eta,w)$ within the objective (3.11) is continuously differentiable with respect to the variables φ, η and w. For the optimal control problem (P), let us introduce now the formal Lagrange function

$$\mathcal{L}(\Phi_{tr}, \Phi_e, W, I_e, P_1, P_2, P_3, P_4, P_5) \,=\, F(\Phi_{tr}, \Phi_e, W, I_e) \,+\, \langle\, P_1\,,\, E_1(\Phi_{tr}, \Phi_e, W)\,\rangle \tag{4.1}$$

$$+\,\langle\, P_2\,,\, E_2(\Phi_{tr}, \Phi_e, I_e)\,\rangle \,+\, \langle\, P_3\,,\, E_3(\Phi_{tr}, W)\,\rangle \,+\, \langle\, P_4\,,\, E_4(\Phi_{tr})\,\rangle \,+\, \langle\, P_5\,,\, E_5(W)\,\rangle$$

with multipliers

$$P_1 \,\in\, L^4\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big]\,; \tag{4.2}$$

$$P_2 \,\in\, L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big] \,\cap\, \Big\{\, Z \;\Big|\; \int_\Omega Z(x,t)\,dx \,=\, 0 \;\; (\forall)\, t \in (\,0\,,\,T\,)\,\Big\}\,; \tag{4.3}$$

$$P_3 \,\in\, L^2\big[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\,\big]\,; P_4,\, P_5 \,\in\, \big(\,L^2(\Omega)\,\big)^*\,. \tag{4.4}$$

Differentiating $\mathcal{L}$ at the point $(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ in a formal way with respect to the variables Φ_{tr}, Φ_e and W, we find the adjoint equations

$$D_{\Phi_{tr}} F\,(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e) \,+\, \langle\, P_1\,,\, D_{\Phi_{tr}}\, E_1(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W})\,\rangle \tag{4.5}$$

$$+\,\langle\, P_2\,,\, D_{\Phi_{tr}}\, E_2(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{I}_e)\,\rangle \,+\, \langle\, P_3\,,\, D_{\Phi_{tr}}\, E_3(\hat{\Phi}_{tr}, \hat{W})\,\rangle \,+\, \langle\, P_4\,,\, D_{\Phi_{tr}}\, E_4(\hat{\Phi}_{tr})\,\rangle \,=\, 0\,;$$

$$D_{\Phi_e} F\,(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e) \,+\, \langle\, P_1\,,\, D_{\Phi_e}\, E_1(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W})\,\rangle \,+\, \langle\, P_2\,,\, D_{\Phi_e}\, E_2(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{I}_e)\,\rangle \,=\, 0\,; \tag{4.6}$$

$$D_W\, F(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e) \,+\, \langle\, P_1\,,\, D_W\, E_1(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W})\,\rangle \,+\, \langle\, P_3\,,\, D_W\, E_3(\hat{\Phi}_{tr}, \hat{W})\,\rangle \,+\, \langle\, P_5\,,\, D_W\, E_5(\hat{W})\,\rangle \,=\, 0\,. \tag{4.7}$$

After choosing $P_4 = -P_1(\cdot\,,0)$ and $P_5 = -P_3(\cdot\,,0)$ (this choice is possible by Theorem 4.2. below), the adjoint system takes the following form:

$$\int_0^T \int_\Omega \Big(-\frac{\partial P_1}{\partial t} + \frac{\partial I_{ion}}{\partial \varphi}(\hat\Phi_{tr}, \hat W)\, P_1 + \frac{\partial G}{\partial \varphi}(\hat\Phi_{tr}, \hat W)\, P_3 \Big)\, \psi\, dx\, dt + \int_0^T \int_\Omega \nabla\psi^{\mathrm T} M_i \,(\, \nabla P_1 + \nabla P_2 \,)\, dx\, dt \quad (4.8)$$
$$= -\int_0^T \int_\Omega \Big(\frac{\partial r}{\partial \varphi}(\hat\Phi_{tr}, \hat\Phi_e, \hat W) \Big)\, \psi\, dx\, dt \quad \forall\, \psi \in L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\big]\,,\ P_1(x,T) \equiv 0\,;$$

$$\int_0^T \int_\Omega \nabla\psi^{\mathrm T} M_i\, \nabla P_1\, dx\, dt + \int_0^T \int_\Omega \nabla\psi^{\mathrm T}\,(M_i + M_e)\, \nabla P_2\, dx\, dt \;=\; -\int_0^T \int_\Omega \frac{\partial r}{\partial \eta}(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\, \psi\, dx\, dt \quad (4.9)$$

$$\forall\, \psi \in L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\big] \text{ with } \int_\Omega \psi(x,t)\, dx = 0 \quad (\forall)\, t \in (\,0\,,\,T\,)\,, \ \int_\Omega P_2(x,t)\, dx = 0 \quad (\forall)\, t \in (\,0\,,\,T\,)\,;$$

$$\int_0^T \int_\Omega \Big(-\frac{\partial P_3}{\partial t} + \frac{\partial I_{ion}}{\partial w}(\hat\Phi_{tr}, \hat W)\, P_1 + \frac{\partial G}{\partial w}(\hat\Phi_{tr}, \hat W)\, P_3 \Big)\, \psi\, dx\, dt \;=\; -\int_0^T \int_\Omega \Big(\frac{\partial r}{\partial w}(\hat\Phi_{tr}, \hat\Phi_e, \hat W) \Big)\, \psi\, dx\, dt \quad (4.10)$$
$$\forall\, \psi \in L^2\big[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\big]\,,\ P_3(x,T) \equiv 0\,.$$

b) The reduced form of the adjoint system.

First, we apply to the system (4.8) − (4.10) the transformation $s = T - t$, thus defining $\widetilde P_i(x,s) = P_i(x, T-s)$, $1 \leqslant i \leqslant 3$, $\widetilde{\Phi_{tr}}(x,s) = \hat\Phi_{tr}(x, T-s)$, $\widetilde{\Phi_e}(x,s) = \hat\Phi_e(x, T-s)$, $\widetilde W(x,s) = \hat W(x, T-s)$ and $\widetilde I_e(x,s) = \hat I_e(x, T-s)$ etc. By abuse of notation, we suppress all tildes, thus simply replacing t by s and $-\partial P_1/\partial t$, $-\partial P_3/\partial t$ by $\partial P_1/\partial s$ and $\partial P_3/\partial s$, respectively. Then the adjoint system, in analogy to the primal bidomain equations, can be rewritten in terms of the bidomain bilinear form as a reduced system:

$$\frac{d}{ds}\langle\, P_1(s)\,,\,\psi\,\rangle + A\big(\,P_1(s)\,,\,\psi\,\big) + \int_\Omega \Big(\frac{\partial I_{ion}}{\partial \varphi}(\hat\Phi_{tr}, \hat W)\, P_1 + \frac{\partial G}{\partial \varphi}(\hat\Phi_{tr}, \hat W)\, P_3 \Big)\, \psi\, dx \;=\; \langle\, \widetilde S(s)\,,\,\psi\,\rangle \quad (4.11)$$
$$\forall\, \psi \in W^{1,2}(\Omega)\,;$$

$$\frac{d}{ds}\langle\, P_3(s)\,,\,\psi\,\rangle + \int_\Omega \Big(\frac{\partial I_{ion}}{\partial w}(\hat\Phi_{tr}, \hat W)\, P_1 + \frac{\partial G}{\partial w}(\hat\Phi_{tr}, \hat W)\, P_3 \Big)\, \psi\, dx \;=\; -\langle\, \frac{\partial r}{\partial w}(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\,,\,\psi\,\rangle \quad (4.12)$$
$$\forall\, \psi \in L^2(\Omega)\,;$$

$$P_1(x,0) \;=\; 0 \quad (\forall)\, x \in \Omega\,; \quad P_3(x,0) \;=\; 0 \quad (\forall)\, x \in \Omega \quad (4.13)$$

on $[\,0\,,\,T\,]$ in distributional sense (cf. [Kunisch/Wagner 11b], p. 5 f., Theorem 2.4. Here the bidomain bilinear form $A\colon\ W^{1,2}(\Omega) \times W^{1,2}(\Omega) \to \mathbb{R}$ is defined as ibid., p. 5, (2.22) through

$$A(\psi_1\,,\,\psi_2) \;=\; \int_\Omega \nabla\psi_1^{\mathrm T} M_i\, \nabla\psi_2\, dx + \int_\Omega \nabla\widetilde\psi_e^{\mathrm T} M_i\, \nabla\psi_2\, dx \quad (4.14)$$

where $\widetilde\psi_e \in W^{1,2}(\Omega)$ is the uniquely determined solution of the variational equation

$$\int_\Omega \nabla\widetilde\psi_e^{\mathrm T}(M_i + M_e)\, \nabla\psi\, dx \;=\; -\int_\Omega \nabla\psi_1^{\mathrm T} M_i\, \nabla\psi\, dx \quad \forall\, \psi \in W^{1,2}(\Omega) \text{ with } \int_\Omega \psi\, dx = 0 \quad (4.15)$$
$$\text{satisfying } \int_\Omega \widetilde\psi_e\, dx \;=\; 0\,,$$

and the linear functionals $\widetilde S(s) \in \big(\,W^{1,2}(\Omega)\,\big)^*$ are defined through

$$\langle\, \widetilde S(s)\,,\,\psi\,\rangle \;=\; -\langle\, \frac{\partial r}{\partial \varphi}(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\,,\,\psi\,\rangle - \int_\Omega \nabla\overline{\psi}_e^{\mathrm T} M_i\, \nabla\psi\, dx \quad (4.16)$$

where $\overline{\psi}_e \in W^{1,2}(\Omega)$ is the uniquely determined solution of the variational equation

$$\int_\Omega \nabla \overline{\psi}_e^{\,\mathrm{T}} (M_i + M_e) \nabla \psi \, dx \;=\; \langle \frac{\partial r}{\partial \eta}(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}) \,,\, \psi \rangle \quad \forall\, \psi \in W^{1,2}(\Omega) \;\text{ with }\; \int_\Omega \psi \, dx = 0 \tag{4.17}$$

$$\text{satisfying } \int_\Omega \overline{\psi}_e \, dx = 0\,.$$

The component P_2 of the solution of (4.8) $-$ (4.10) is uniquely determined as the sum $P_2 = \widetilde{\psi}_e + \overline{\psi}_e$. Note that this reformulation is even possible without imposing the additional compatibility condition

$$\int_\Omega \frac{\partial r}{\partial \eta}\big(\, \hat{\Phi}_{tr}(x,s), \hat{\Phi}_e(x,s), \hat{W}(x,s) \,\big)\, dx \;=\; 0 \quad (\forall)\, s \in (\, 0\,,\, T\,)\,. \tag{4.18}$$

c) Existence of weak solutions.

Theorem 4.1. (A-priori estimates for weak solutions of the adjoint system) *The optimal control problem* (P) *is studied under the assumptions from Subsection 3.a). Within the problem, any of the three models from Subsection 2.b) is specified. Assume further that the integrand $r(x,t,\varphi,\eta,w)$ is continuously differentiable with respect to φ, η and w. If $(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ is a feasible solution of* (P) *with*

$$\frac{\partial r}{\partial \varphi}(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W})\,,\; \frac{\partial r}{\partial \eta}(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W})\,,\; \frac{\partial r}{\partial w}(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}) \in L^4\big[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\,\big]\,; \tag{4.19}$$

then every weak solution $(P_1, P_2, P_3) \in L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big] \times L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big] \times L^2(\Omega_T)$ of the adjoint system (4.8) $-$ (4.10) *obeys the estimate*

$$\begin{aligned} \|\, P_1 \,\|^2_{C^0[\,[\,0\,,\,T\,]\,,\,L^2(\Omega)\,]} + \|\, P_1 \,\|^4_{L^4[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,]} + \|\, \partial P_1/\partial s \,\|^2_{L^2[\,(\,0\,,\,T\,)\,,\,(\,W^{1,2}(\Omega)\,)^*\,]} \\ + \|\, P_2 \,\|^2_{L^2[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,]} + \|\, P_3 \,\|^2_{C^0[\,[\,0\,,\,T\,]\,,\,L^2(\Omega)\,]} + \|\, \partial P_3/\partial s \,\|^2_{L^2(\Omega_T)} \leqslant C \end{aligned} \tag{4.20}$$

where the constant $C > 0$ does not depend on P_1, P_2, P_3 but on $(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ and the data of (P).

Assumption (4.19) about $\partial r(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W})/\partial \eta$ is rather restrictive since, in general, only $\hat{\Phi}_e \in L^2\big[\,(\,0\,,\,T\,)\,,\, W^{1,2}(\Omega)\,\big]$ can be guaranteed. [11] In fact, the bidomain system does not allow for smoothing of Φ_e or Φ_i in time but only of Φ_{tr}.
The a-priori estimates yield the following existence theorem for the adjoint system:

Theorem 4.2. (Existence of solutions for the adjoint system) *Under the assumptions of Theorem 4.1., the adjoint system* (4.8) $-$ (4.10) *admits a weak solution (P_1, P_2, P_3) with*

$$P_1 \in C^0\big[\,[\,0\,,\,T\,]\,,\,L^2(\Omega)\,\big] \cap L^4\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big]\,; \tag{4.21}$$

$$P_2 \in L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big]\,; \quad \int_\Omega P_2(x,t)\, dx = 0 \;\; (\forall)\, t \in (\,0\,,\,T\,)\,; \tag{4.22}$$

$$P_3 \in C^0\big[\,[\,0\,,\,T\,]\,,\,L^2(\Omega)\,\big]\,. \tag{4.23}$$

Proof of Theorem 4.1. Throughout the proof, C denotes a generical positive constant, which may appropriately change from line to line. Further, we will specify in (3.12) $-$ (3.14) the Rogers-McCulloch model. The necessary alterations in the case of the other models will be discussed at the end of the proof.

---

[11] An example of a functional satisfying (4.19) is given by $\dfrac{1}{2}\displaystyle\int_\Omega \Big(\frac{1}{2\,\varepsilon} \int_{t-\varepsilon}^{t+\varepsilon} \Phi_e(x,\tau)\, d\tau - \Phi_{ref}(x) \Big)^2 dx$.

• **Step 1.** *Since* $\hat{I}_e \in L^\infty\big[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\,\big]$, *it holds that* $\hat{\Phi}_{tr} \in L^\infty\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big]$ *and* $\hat{W} \in C^0\big[\,[\,0\,,\,T\,]\,,\,L^4(\Omega)\,\big]$. In fact, we rely on the estimate [Kunisch/Wagner 11b], p. 22, (3.31), which reads after the insertion of $I_i = \mathfrak{o}$ as follows:

$$\|\,\hat{\Phi}_{tr}(t)\,\|^2_{W^{1,2}(\Omega)} \leqslant C\,\Big(\,1 + \|\,\Phi_0\,\|^2_{L^2(\Omega)} + \|\,W_0\,\|^2_{L^2(\Omega)} + \|\,\hat{I}_e(t)\,\|^2_{L^2(\Omega)} + \int_0^t \|\,\hat{I}_e(\tau)\,\|^2_{\big(W^{1,2}(\Omega)\big)^*}\,d\tau\,\Big) \tag{4.24}$$

$$\leqslant C\,\Big(\,1 + \|\,\Phi_0\,\|^2_{L^2(\Omega)} + \|\,W_0\,\|^2_{L^2(\Omega)} + (1+T)\,\|\,\hat{I}_e\,\|^2_{L^\infty\big[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\,\big]}\,\Big) \tag{4.25}$$

for arbitrary $t \in (\,0\,,\,T\,)$. Thus the claimed regularity of $\hat{\Phi}_{tr}$ is confirmed. Note that

$$\hat{W}(x,t) \,=\, W_0(x)\,e^{-\varepsilon t} + \varepsilon\,\kappa \int_0^t \hat{\Phi}_{tr}(x,\tau)\,e^{\varepsilon(\tau-t)}\,d\tau\,, \tag{4.26}$$

belongs to $C^0\big[\,[\,0\,,\,T\,]\,,\,L^4(\Omega)\,\big]$ together with $\hat{\Phi}_{tr}(\,\cdot\,,\tau)$, $W_0 \in L^4(\Omega)$.

• **Step 2.** *An estimate for the right-hand side of* (4.11). We start with

Lemma 4.3. *Under the assumptions of Theorem 4.1., for arbitrary* $\varepsilon > 0$ *the following estimate holds:*

$$\big|\,\langle\,\widetilde{S}(s)\,,\,\psi\,\rangle\,\big| \,\leqslant\, \frac{C}{2\varepsilon}\,\Big(\,\|\,\frac{\partial r}{\partial\varphi}(\hat{\Phi}_{tr},\hat{\Phi}_e,\hat{W})\,\|^2_{L^2(\Omega)} + \|\,\frac{\partial r}{\partial\eta}(\hat{\Phi}_{tr},\hat{\Phi}_e,\hat{W})\,\|^2_{L^2(\Omega)}\,\Big) + \frac{3\varepsilon}{4}\,\|\,\psi\,\|^2_{W^{1,2}(\Omega)}\,. \tag{4.27}$$

The constant $C > 0$ *does not depend on* ε *and* ψ.

Proof. Inserting $\overline{\psi}_e \in W^{1,2}(\Omega)$ as a feasible test function into (4.17), we get from the uniform ellipticity of M_i and M_e and the Poincaré inequality:

$$C\,\|\,\overline{\psi}_e\,\|^2_{W^{1,2}(\Omega)} \,\leqslant\, \int_\Omega \nabla\overline{\psi}_e^{\,\mathrm{T}}(M_i + M_e)\,\nabla\overline{\psi}_e^{\,\mathrm{T}}\,dx \,\leqslant\, \big|\,\langle\,\frac{\partial r}{\partial\eta}(\hat{\Phi}_{tr},\hat{\Phi}_e,\hat{W})\,,\,\overline{\psi}_e^{\,\mathrm{T}}\,\rangle\big| \tag{4.28}$$

$$\leqslant\, \frac{1}{2\varepsilon}\,\|\,\frac{\partial r}{\partial\eta}(\hat{\Phi}_{tr},\hat{\Phi}_e,\hat{W})\,\|^2_{\big(W^{1,2}(\Omega)\big)^*} + \frac{\varepsilon}{2}\,\|\,\overline{\psi}_e\,\|^2_{W^{1,2}(\Omega)} \quad (\forall)\,s \in (\,0\,,\,T\,)\,,$$

and with $\varepsilon = C/2$, we arrive at

$$\frac{C}{2}\,\|\,\overline{\psi}_e\,\|^2_{W^{1,2}(\Omega)} \,\leqslant\, \frac{1}{C}\,\|\,\frac{\partial r}{\partial\eta}(\hat{\Phi}_{tr},\hat{\Phi}_e,\hat{W})\,\|^2_{\big(W^{1,2}(\Omega)\big)^*} \,\leqslant\, \frac{1}{C}\,\|\,\frac{\partial r}{\partial\eta}(\hat{\Phi}_{tr},\hat{\Phi}_e,\hat{W})\,\|^2_{L^2(\Omega)}\,. \tag{4.29}$$

From (4.16), we obtain

$$\big|\,\langle\,\widetilde{S}(s)\,,\,\psi\,\rangle\,\big| \,\leqslant\, \big|\,\langle\,\frac{\partial r}{\partial\varphi}(\hat{\Phi}_{tr},\hat{\Phi}_e,\hat{W})\,,\,\psi\,\rangle\,\big| + \big|\,\langle\,\nabla\overline{\psi}_e^{\,\mathrm{T}} M_i\,,\,\nabla\psi\,\rangle\,\big| \tag{4.30}$$

$$\leqslant\, \frac{1}{2\varepsilon}\,\|\,\frac{\partial r}{\partial\varphi}(\hat{\Phi}_{tr},\hat{\Phi}_e,\hat{W})\,\|^2_{\big(W^{1,2}(\Omega)\big)^*} + \frac{\varepsilon}{2}\,\|\,\psi\,\|^2_{W^{1,2}(\Omega)} + \frac{1}{2\varepsilon'}\,\|\,\overline{\psi}_e\,\|^2_{L^2(\Omega)} + \frac{\varepsilon'}{2}\,\|\,M_i\,\|^2\cdot\|\,\psi\,\|^2_{L^2(\Omega)} \tag{4.31}$$

$$\leqslant\, \frac{1}{2\varepsilon}\,\|\,\frac{\partial r}{\partial\varphi}(\hat{\Phi}_{tr},\hat{\Phi}_e,\hat{W})\,\|^2_{L^2(\Omega)} + \frac{1}{2\varepsilon'}\,\|\,\overline{\psi}_e\,\|^2_{W^{1,2}(\Omega)} + \Big(\,\frac{\varepsilon}{2} + \frac{(\mu_2)^2\,\varepsilon'}{2}\,\Big)\,\|\,\psi\,\|^2_{W^{1,2}(\Omega)} \tag{4.32}$$

$$\leqslant\, \frac{1}{2\varepsilon}\,\|\,\frac{\partial r}{\partial\varphi}(\hat{\Phi}_{tr},\hat{\Phi}_e,\hat{W})\,\|^2_{L^2(\Omega)} + \frac{C}{2\varepsilon'}\,\|\,\frac{\partial r}{\partial\eta}(\hat{\Phi}_{tr},\hat{\Phi}_e,\hat{W})\,\|^2_{L^2(\Omega)} + \Big(\,\frac{\varepsilon}{2} + \frac{(\mu_2)^2\varepsilon'}{2}\,\Big)\,\|\,\psi\,\|^2_{W^{1,2}(\Omega)} \tag{4.33}$$

by (2.5) and (4.29). Taking $\varepsilon' = \varepsilon/(2\,(\mu_2)^2)$, we get (4.27). ∎

• **Step 3.** *The estimates for* $\|\,P_1\,\|_{L^\infty\big[\,[\,0\,,\,T\,]\,,\,L^2(\Omega)\,\big]}$ *and* $\|\,P_3\,\|_{L^\infty\big[\,[\,0\,,\,T\,]\,,\,L^2(\Omega)\,\big]}$. Specifying the derivatives of I_{ion} and G according to the Rogers-McCulloch model, we have

$$\frac{\partial I_{ion}}{\partial\varphi}(\hat{\Phi}_{tr},\hat{W}) \,=\, 3\,b\,(\hat{\Phi}_{tr})^2 - 2\,(a+1)\,b\,\hat{\Phi}_{tr} + ab + \hat{W}\,; \quad \frac{\partial G}{\partial\varphi}(\hat{\Phi}_{tr},\hat{W}) \,\equiv\, -\varepsilon\,\kappa\,; \tag{4.34}$$

$$\frac{\partial I_{ion}}{\partial w}(\hat{\Phi}_{tr},\hat{W}) \,=\, \hat{\Phi}_{tr}\,; \quad \frac{\partial G}{\partial w}(\hat{\Phi}_{tr},\hat{W}) \,\equiv\, \varepsilon\,. \tag{4.35}$$

Inserting $P_1(s)$ as a feasible test function into (4.11), we get for arbitrary $\varepsilon_1, \varepsilon_2 > 0$ with [Kunisch/Wagner 11b] , p. 6, Theorem 2.4., 2), and Lemma 4.3. above

$$\frac{1}{2}\frac{d}{ds}\,\|\,P_1(s)\,\|^2_{L^2(\Omega)} + \Big(A(P_1,P_1) + \beta\,\|\,P_1\,\|^2_{L^2(\Omega)} \Big) \tag{4.36}$$
$$\leqslant \int_\Omega \Big|\,\frac{\partial I_{ion}}{\partial\varphi}(\hat\Phi_{tr},\hat W)\,\Big|\,|\,P_1\,|^2\,dx + \int_\Omega \Big|\,\frac{\partial G}{\partial\varphi}(\hat\Phi_{tr},\hat W)\,\Big|\,|\,P_1\,P_3\,| + |\,\langle\,\widetilde S(s)\,,\,P_1\,\rangle\,| + \beta\,\|\,P_1\,\|^2_{L^2(\Omega)} \quad\Longrightarrow$$

$$\frac{1}{2}\frac{d}{ds}\,\|\,P_1(s)\,\|^2_{L^2(\Omega)} + \beta\,\|\,P_1\,\|^2_{W^{1,2}(\Omega)}$$
$$\leqslant C\int_\Omega \Big(\,|\,\hat\Phi_{tr}\,|^2 + |\,\hat\Phi_{tr}\,| + |\,\hat W\,| + 1\Big)\,|\,P_1\,|^2\,dx + \varepsilon\,\kappa\int_\Omega |\,P_1\,P_3\,|\,dx \tag{4.37}$$
$$+\ \frac{C}{2\varepsilon_1}\Big(\|\,\frac{\partial r}{\partial\varphi}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)} + \|\,\frac{\partial r}{\partial\eta}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)}\Big) + \frac{3\varepsilon_1}{4}\,\|\,P_1\,\|^2_{W^{1,2}(\Omega)} + \beta\,\|\,P_1\,\|^2_{L^2(\Omega)}$$

$$\leqslant \frac{C\,\varepsilon_2}{2}\int_\Omega \Big(\,|\,\hat\Phi_{tr}\,|^2 + |\,\hat\Phi_{tr}\,| + |\,\hat W\,| + 1\Big)^2\,|\,P_1\,|^2\,dx + \Big(\frac{C}{2\,\varepsilon_2} + 3\,\varepsilon\,\kappa + \beta\Big)\,\|\,P_1\,\|^2_{L^2(\Omega)} \tag{4.38}$$
$$+\,3\,\varepsilon\,\kappa\,\|\,P_3\,\|^2_{L^2(\Omega)} + \frac{C}{2\varepsilon_1}\Big(\|\,\frac{\partial r}{\partial\varphi}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)} + \|\,\frac{\partial r}{\partial\eta}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)}\Big) + \frac{3\varepsilon_1}{4}\,\|\,P_1\,\|^2_{W^{1,2}(\Omega)}$$

$$\leqslant \frac{C\,\varepsilon_2}{2}\Big(\int_\Omega\Big(\,|\,\hat\Phi_{tr}\,|^2 + |\,\hat\Phi_{tr}\,| + |\,\hat W\,| + 1\Big)^3\,dx\Big)^{2/3}\cdot\Big(\int_\Omega |\,P_1\,|^6\,dx\Big)^{1/3} + \Big(\frac{C}{2\,\varepsilon_2} + 3\,\varepsilon\,\kappa + \beta\Big)\,\|\,P_1\,\|^2_{L^2(\Omega)} \tag{4.39}$$
$$+\ 3\,\varepsilon\,\kappa\,\|\,P_3\,\|^2_{L^2(\Omega)} + \frac{C}{2\varepsilon_1}\Big(\|\,\frac{\partial r}{\partial\varphi}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)} + \|\,\frac{\partial r}{\partial\eta}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)}\Big) + \frac{3\varepsilon_1}{4}\,\|\,P_1\,\|^2_{W^{1,2}(\Omega)}\,.$$

From Step 1 we know that $\hat\Phi_{tr}(s) \in W^{1,2}(\Omega) \hookrightarrow L^6(\Omega)$ and $\hat W(s) \in L^4(\Omega)$ for all $s \in (\,0\,,T\,)$, and the respective norms are essentially bounded. Thus we get

$$\int_\Omega\Big(\,|\,\hat\Phi_{tr}(s)\,|^2 + |\,\hat\Phi_{tr}(s)\,| + |\,\hat W(s)\,| + 1\Big)^3\,dx \;\leqslant\; C\,\Big(\,\|\,\hat\Phi_{tr}(s)\,\|^6_{L^6(\Omega)} + \|\,\hat\Phi_{tr}(s)\,\|^3_{L^3(\Omega)} + \|\,\hat W(s)\,\|^3_{L^3(\Omega)} + 1\Big) \;\leqslant\; C\,, \tag{4.40}$$

and estimate (4.39) can be continued as follows:

$$\frac{1}{2}\frac{d}{ds}\,\|\,P_1(s)\,\|^2_{L^2(\Omega)} + \beta\,\|\,P_1\,\|^2_{W^{1,2}(\Omega)} \;\leqslant\; C\,\varepsilon_2\,\|\,P_1\,\|^2_{L^6(\Omega)} + \Big(\frac{C}{2\,\varepsilon_2} + 3\,\varepsilon\,\kappa + \beta\Big)\,\|\,P_1\,\|^2_{L^2(\Omega)} \tag{4.41}$$
$$+\ 3\,\varepsilon\,\kappa\,\|\,P_3\,\|^2_{L^2(\Omega)} + \frac{C}{2\varepsilon_1}\Big(\|\,\frac{\partial r}{\partial\varphi}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)} + \|\,\frac{\partial r}{\partial\eta}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)}\Big) + \frac{3\varepsilon_1}{4}\,\|\,P_1\,\|^2_{W^{1,2}(\Omega)}$$

$$\leqslant \Big(\,\frac{3\,\varepsilon_1}{4} + C\,\varepsilon_2\Big)\,\|\,P_1\,\|^2_{W^{1,2}(\Omega)} + C\,\Big(1 + \frac{1}{2\,\varepsilon_2}\Big)\,\|\,P_1\,\|^2_{L^2(\Omega)} + C\,\|\,P_3\,\|^2_{L^2(\Omega)} \tag{4.42}$$
$$+\ \frac{C}{2\varepsilon_1}\Big(\|\,\frac{\partial r}{\partial\varphi}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)} + \|\,\frac{\partial r}{\partial\eta}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)}\Big)\,.$$

Further, inserting P_3 as a feasible test function into (4.12), we find

$$\frac{1}{2}\frac{d}{ds}\,\|\,P_3\,\|^2_{L^2(\Omega)}$$
$$\leqslant \int_\Omega \Big|\,\frac{\partial I_{ion}}{\partial w}(\hat\Phi_{tr},\hat W)\,\Big|\,|\,P_1\,P_3\,|\,dx + \int_\Omega \Big|\,\frac{\partial G}{\partial w}(\hat\Phi_{tr},\hat W)\,\Big|\,|\,P_3\,|^2\,dx + \int_\Omega \Big|\,\frac{\partial r}{\partial w}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\Big|\,|P_3\,|\,dx \tag{4.43}$$
$$\leqslant \int_\Omega |\,\hat\Phi_{tr}\,P_1\,P_3\,|\,dx + \varepsilon\,\|\,P_3\,\|^2_{L^2(\Omega)} + C\,\|\,\frac{\partial r}{\partial w}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)} + C\,\|\,P_3\,\|^2_{L^2(\Omega)} \tag{4.44}$$
$$\leqslant \frac{\varepsilon_3}{2}\int_\Omega |\,\hat\Phi_{tr}\,P_1\,|^2\,dx + \Big(\frac{1}{2\,\varepsilon_3} + \varepsilon + C\Big)\,\|\,P_3\,\|^2_{L^2(\Omega)} + C\,\|\,\frac{\partial r}{\partial w}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)} \tag{4.45}$$
$$\leqslant \frac{C\,\varepsilon_3}{2}\,\|\,P_1\,\|^2_{W^{1,2}(\Omega)} + \Big(\frac{1}{2\,\varepsilon_3} + \varepsilon + C\Big)\,\|\,P_3\,\|^2_{L^2(\Omega)} + C\,\|\,\frac{\partial r}{\partial w}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)}\,. \tag{4.46}$$

Combining (4.42) and (4.46), we obtain

$$\frac{d}{ds}\Big(\,\|\,P_1(s)\,\|^2_{L^2(\Omega)}+\|\,P_3(s)\,\|^2_{L^2(\Omega)}\Big)+2\,\beta\,\|\,P_1\,\|^2_{W^{1,2}(\Omega)} \tag{4.47}$$
$$\leqslant\Big(\,\frac{3\,\varepsilon_1}{2}+2\,C\,\varepsilon_2+C\,\varepsilon_3\Big)\,\|\,P_1\,\|^2_{W^{1,2}(\Omega)}+C\,\Big(2+\frac{1}{\varepsilon_2}\Big)\,\|\,P_1\,\|^2_{L^2(\Omega)}+\Big(\,\frac{1}{\varepsilon_3}+2\,\varepsilon+4\,C\Big)\,\|\,P_3\,\|^2_{L^2(\Omega)}$$
$$+\;\frac{C}{\varepsilon_1}\Big(\,\|\,\frac{\partial r}{\partial\varphi}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)}+\|\,\frac{\partial r}{\partial\eta}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)}\Big)+2\,C\,\|\,\frac{\partial r}{\partial w}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)}\,.$$

Now we fix the parameters $\varepsilon_1,\,\varepsilon_2,\,\varepsilon_3>0$ in such a way that the terms with $\|\,P_1\,\|_{W^{1,2}(\Omega)}$ annihilate. After majorizing the factors on the right-hand side by a uniform constant, Gronwall's inequality yields for all $s\in[\,0\,,\,T\,]$:

$$\|\,P_1(s)\,\|^2_{L^2(\Omega)}+\|\,P_3(s)\,\|^2_{L^2(\Omega)}\;\leqslant\;e^{Cs}\,\Big(\,\|\,P_1(0)\,\|^2_{L^2(\Omega)}+\|\,P_3(0)\,\|^2_{L^2(\Omega)} \tag{4.48}$$
$$+\int_0^s\Big(\,\|\,\frac{\partial r}{\partial\varphi}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)}+\|\,\frac{\partial r}{\partial\eta}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)}+\|\,\frac{\partial r}{\partial w}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)}\Big)\,ds\Big)$$
$$\leqslant\;e^{CT}\,\Big(\,\|\,\frac{\partial r}{\partial\varphi}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega_T)}+\|\,\frac{\partial r}{\partial\eta}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega_T)}+\|\,\frac{\partial r}{\partial w}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega_T)}\Big)\,. \tag{4.49}$$

Consequently, we get the estimate

$$\|\,P_1\,\|^2_{L^\infty\left[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\right]}+\|\,P_3\,\|^2_{L^\infty\left[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\right]}\;\leqslant\;C\,\Big(\,\|\,\frac{\partial r}{\partial\varphi}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega_T)} \tag{4.50}$$
$$+\,\|\,\frac{\partial r}{\partial\eta}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega_T)}+\|\,\frac{\partial r}{\partial w}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega_T)}\Big)\,.$$

• **Step 4.** *The estimate for* $\|\,P_1\,\|^4_{L^4\left[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\right]}$. We return to (4.47). Choosing $\varepsilon_1,\,\varepsilon_2,\,\varepsilon_3>0$ according to $3\,\varepsilon_1/2+2\,C\,\varepsilon_2+C\,\varepsilon_3\;=\;\beta$ and equalizing the constants on the right-hand side, we get the following inequality:

$$\beta\,\|\,P_1(s)\,\|^2_{W^{1,2}(\Omega)}\;\leqslant\;C\,\Big(\,\|\,P_1(s)\,\|^2_{L^2(\Omega)}+\|\,P_3(s)\,\|^2_{L^2(\Omega)} \tag{4.51}$$
$$+\,\|\,\frac{\partial r}{\partial\varphi}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)}+\|\,\frac{\partial r}{\partial\eta}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)}+\|\,\frac{\partial r}{\partial w}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)}\Big)\,.$$

Inserting (4.50) into (4.51), we arrive at

$$\|\,P_1(s)\,\|^2_{W^{1,2}(\Omega)}\;\leqslant\;C\,\Big(\,\|\,\frac{\partial r}{\partial\varphi}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega_T)}+\|\,\frac{\partial r}{\partial\eta}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega_T)}+\|\,\frac{\partial r}{\partial w}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega_T)}$$
$$+\;\|\,\frac{\partial r}{\partial\varphi}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)}+\|\,\frac{\partial r}{\partial\eta}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)}+\|\,\frac{\partial r}{\partial w}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^2_{L^2(\Omega)}\Big)\quad\Longrightarrow \tag{4.52}$$

$$\|\,P_1\,\|^4_{L^4\left[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\right]}\;=\;\int_0^T\|\,P_1(s)\,\|^4_{W^{1,2}(\Omega)}\,ds\;\leqslant\;C\,\Big(1+\|\,\frac{\partial r}{\partial\varphi}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^4_{L^4\left[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\right]}$$
$$+\,\|\,\frac{\partial r}{\partial\eta}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^4_{L^4\left[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\right]}+\|\,\frac{\partial r}{\partial w}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,\|^4_{L^4\left[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\right]}\Big)\,. \tag{4.53}$$

• **Step 5.** *The estimate for* $\|\,\partial P_1/\partial s\,\|^2_{L^2\left[\,(\,0\,,\,T\,)\,,\,\left(\,W^{1,2}(\Omega)\right)^*\right]}$. Exploiting the definition of the dual norm, we start with

$$\|\,\partial P_1/\partial s\,\|^2_{L^2\left[\,(\,0\,,\,T\,)\,,\,\left(\,W^{1,2}(\Omega)\right)^*\right]}\;=\;\int_0^T\sup_{\|\,\psi\,\|_{W^{1,2}(\Omega)}\,=\,1}\big|\,\langle\,\partial P_1(s)/\partial s\,,\,\psi\,\rangle\,\big|^2\,ds \tag{4.54}$$

$$=\;\int_0^T\sup_{\cdots}\Big|-A(P_1,\psi)-\int_\Omega\Big(\frac{\partial I_{ion}}{\partial\varphi}(\hat\Phi_{tr},\hat W)\,P_1+\frac{\partial G}{\partial\varphi}(\hat\Phi_{tr},\hat W)\,P_3\Big)\,\psi\,dx+\langle\,\widetilde S(s)\,,\,\psi\,\rangle\Big|^2\,ds \tag{4.55}$$

$$\leqslant\;C\int_0^T\Big(\sup_{\cdots}\big|\,A(P_1,\psi)\,\big|^2+\sup_{\cdots}\Big(\int_\Omega\Big(\,\big|\,\hat\Phi_{tr}\,\big|^2+\big|\,\hat\Phi_{tr}\,\big|+\big|\,\hat W\,\big|+1\Big)\,\big|\,P_1\,\big|\,\big|\,\psi\,\big|\,dx\Big)^2 \tag{4.56}$$
$$+\,\sup_{\cdots}\,\varepsilon^2\,\kappa^2\,\Big(\int_\Omega\big|\,P_3\,\big|\,\big|\,\psi\,\big|\,dx\Big)^2+\sup_{\cdots}\big|\,\langle\,\widetilde S(s)\,,\,\psi\,\rangle\,\big|^2\Big)\,ds\,.$$

The four terms on the right-hand side of (4.56) will be estimated separately. For the first term, we get with [Kunisch/Wagner 11b] , p. 6, Theorem 2.4., 2):

$$\int_0^T \sup_{\dots} \big|\, A(P_1,\psi)\,\big|^2\, ds \leqslant \int_0^T \sup_{\dots} \gamma^2\, \|\, P_1(s)\,\|^2_{W^{1,2}(\Omega)}\, \|\,\psi\,\|^2_{W^{1,2}(\Omega)}\, ds \leqslant \gamma^2\, \|\, P_1\,\|^2_{L^2\left[\,(0,T),\, W^{1,2}(\Omega)\,\right]}\,, \tag{4.57}$$

which is bounded by (4.53). For the second term, we obtain

$$\int_0^T \sup_{\dots} \Big(\int_\Omega \Big(\,|\, \hat\Phi_{tr}\,|^2 + |\,\hat\Phi_{tr}\,| + |\,\hat W\,| + 1 \Big)\, |\, P_1\,|\,|\,\psi\,|\, dx \Big)^2 ds \tag{4.58}$$

$$\leqslant \int_0^T \sup_{\dots} \Big(\int_\Omega \Big(\,|\, \hat\Phi_{tr}\,|^2 + |\,\hat\Phi_{tr}\,| + |\,\hat W\,| + 1 \Big)^2 dx \Big) \cdot \Big(\int_\Omega |\, P_1\,|^3\, dx \Big)^{2/3} \cdot \Big(\int_\Omega |\,\psi\,|^6\, dx \Big)^{1/3} ds\,.$$

Analogously to (4.40), the first factor on the right-hand side of (4.58) may be estimated by a constant, and we get (4.59)

$$\int_0^T \sup_{\dots} \Big(\int_\Omega \Big(\,|\, \hat\Phi_{tr}\,|^2 + |\,\hat\Phi_{tr}\,| + |\,\hat W\,| + 1 \Big)\, |\, P_1\,|\,|\,\psi\,|\, dx \Big)^2 ds \leqslant \int_0^T \sup_{\dots} \Big(C \cdot \|\, P_1(s)\,\|_{L^3(\Omega)} \cdot \|\,\psi\,\|_{L^6(\Omega)} \Big)^2 ds$$

$$\leqslant \int_0^T \sup_{\dots} \Big(C \cdot \|\, P_1(s)\,\|_{W^{1,2}(\Omega)} \cdot \|\,\psi\,\|_{W^{1,2}(\Omega)} \Big)^2 ds \leqslant C\, \|\, P_1\,\|^2_{L^2\left[\,(0,T),\, W^{1,2}(\Omega)\,\right]}\,, \tag{4.60}$$

which is bounded again by (4.53). The third term will be estimated by means of

$$\int_0^T \sup_{\dots} \varepsilon^2\, \kappa^2 \Big(\int_\Omega |\, P_3\,|\,|\,\psi\,|\, dx \Big)^2 ds \leqslant C \int_0^T \sup_{\dots}\ \|\, P_3(s)\,\|^2_{L^2(\Omega)} \cdot \|\,\psi\,\|^2_{L^2(\Omega)}\, ds \tag{4.61}$$

$$\leqslant C \int_0^T \sup_{\dots}\ \|\, P_3(s)\,\|^2_{L^2(\Omega)} \cdot \|\,\psi\,\|^2_{W^{1,2}(\Omega)}\, ds \leqslant C\, \|\, P_3\,\|^2_{L^2(\Omega_T)}\,, \tag{4.62}$$

which is bounded by (4.50). Finally, applying Lemma 4.3. with $\varepsilon = 1$, we get for the last term

$$\int_0^T \sup_{\dots} \big|\, \langle\, \widetilde S(s)\,,\, \psi\,\rangle\,\big|^2\, ds$$

$$\leqslant \int_0^T \sup_{\dots} \Big(\frac{C}{2} \Big(\|\, \frac{\partial r}{\partial \varphi}(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\,\|^2_{L^2(\Omega)} + \|\, \frac{\partial r}{\partial \eta}(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\,\|^2_{L^2(\Omega)} \Big) + \frac{3}{4}\, \|\,\psi\,\|^2_{W^{1,2}(\Omega)} \Big)^2 ds \tag{4.63}$$

$$\leqslant C \Big(1 + \|\, \frac{\partial r}{\partial \varphi}(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\,\|^4_{L^4\left[\,(0,T),\, L^2(\Omega)\,\right]} + \|\, \frac{\partial r}{\partial \eta}(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\,\|^4_{L^4\left[\,(0,T),\, L^2(\Omega)\,\right]} \Big)\,. \tag{4.64}$$

By assumption of the theorem, the right-hand side is bounded as well. Summing up, from (4.57), (4.60), (4.62) and (4.64), we get the claimed bound for $\|\, \partial P_1/\partial s\,\|^2_{L^2\left[\,(0,T),\, \left(W^{1,2}(\Omega)\right)^*\,\right]}$.

• **Step 6.** *The estimate for* $\|\, \partial P_3/\partial s\,\|^2_{L^2(\Omega_T)}$. We start again by using the dual norm:

$$\|\, \partial P_3/\partial s\,\|^2_{L^2(\Omega_T)} = \|\, \partial P_3/\partial s\,\|^2_{L^2\left[\,(0,T),\, \left(L^2(\Omega)\right)^*\,\right]} = \int_0^T \sup_{\|\,\psi\,\|_{L^2(\Omega)} = 1} \big|\, \langle\, \partial P_3(s)/\partial s\,,\, \psi\,\rangle\,\big|^2\, ds \tag{4.65}$$

$$= \int_0^T \sup_{\dots} \Big|\, \int_\Omega \Big(-\frac{\partial I_{ion}}{\partial w}(\hat\Phi_{tr}, \hat W)\, P_1 - \frac{\partial G}{\partial w}(\hat\Phi_{tr}, \hat W)\, P_3 - \frac{\partial r}{\partial w}(\hat\Phi_{tr}, \hat\Phi_e, \hat W) \Big)\, \psi\, dx\,\Big|^2 ds \tag{4.66}$$

$$\leqslant C \int_0^T \sup_{\dots} \Big(\Big(\int_\Omega |\, \hat\Phi_{tr}\,|\,|\, P_1\,|\,|\,\psi\,|\, dx \Big)^2 + \Big(\varepsilon \int_\Omega |P_3\,|\,|\,\psi\,|\, dx \Big)^2 \tag{4.67}$$

$$+ \Big(\int_\Omega |\, \frac{\partial r}{\partial w}(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\,|\,|\,\psi\,|\, dx \Big)^2 \Big) ds$$

$$\leqslant C \int_0^T \Big(\sup_{\dots} \|\, \hat\Phi_{tr}(s)\,\|^2_{L^4(\Omega)} \cdot \|\, P_1\,\|^2_{L^4(\Omega)} \cdot \|\,\psi\,\|^2_{L^2(\Omega)} + \sup_{\dots} \|\, P_3\,\|^2_{L^2(\Omega)} \cdot \|\,\psi\,\|^2_{L^2(\Omega)} \tag{4.68}$$

$$+ \sup_{\dots} \|\, \frac{\partial r}{\partial w}(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\,\|^2_{L^2(\Omega)} \cdot \|\,\psi\,\|^2_{L^2(\Omega)} \Big) ds$$

$$\leqslant C \int_0^T \Big(\|\, \hat\Phi_{tr}(s)\,\|^2_{L^4(\Omega)} \cdot \|\, P_1\,\|^2_{W^{1,2}(\Omega)} + \|\, P_3\,\|^2_{L^2(\Omega)} + \|\, \frac{\partial r}{\partial w}(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\,\|^2_{L^2(\Omega)} \Big) ds\,. \tag{4.69}$$

By Step 1, the norms $\| \hat{\Phi}_{tr}(s) \|_{L^4(\Omega)}$ are essentially bounded. Consequently, we get

$$\| \partial P_3/\partial s \|^2_{L^2(\Omega_T)} \leqslant C \Big(\| P_1 \|^2_{L^2\left[(0,T), W^{1,2}(\Omega)\right]} + \| P_3 \|^2_{L^2(\Omega_T)} + \| \frac{\partial r}{\partial w}(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}) \|^2_{L^2(\Omega_T)} \Big), \tag{4.70}$$

and the claimed bound follows from (4.50) and (4.53).

• **Step 7.** *The estimate for* $\| P_2 \|^2_{L^2\left[(0,T), W^{1,2}(\Omega)\right]}$. Inserting $P_2(s) \in W^{1,2}(\Omega)$ with $\int_\Omega P_2(x,s)\,dx = 0$ as a feasible test function into (4.9), the uniform ellipticity of M_i, M_e and the Poincaré inequality imply

$$\| P_2(s) \|^2_{W^{1,2}(\Omega)} \leqslant C \int_\Omega \nabla P_2^{\mathrm{T}} (M_i + M_e) \nabla P_2 \, dx \tag{4.71}$$

$$\leqslant C \Big(\int_\Omega \nabla P_2^{\mathrm{T}} M_i \nabla P_1 \, dx + \int_\Omega \frac{\partial r}{\partial \eta}(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}) P_2 \, dx \Big) \tag{4.72}$$

$$\leqslant C \Big(\| P_2 \|_{W^{1,2}(\Omega)} \cdot \| P_1 \|_{\left(W^{1,2}(\Omega)\right)^*} + \big| \langle \frac{\partial r}{\partial \eta}(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}), P_2 \rangle_{L^2(\Omega), L^2(\Omega)} \big| \Big) \tag{4.73}$$

since, by Assumption 2.1., 2), the entries of M_i are essentially bounded. Consequently, applying the generalized Cauchy inequality twice, we get

$$\| P_2(s) \|^2_{W^{1,2}(\Omega)} \leqslant C \Big(\frac{1}{2\varepsilon_4} \| \nabla P_1 \|^2_{\left(W^{1,2}(\Omega)\right)^*} + \frac{\varepsilon_4}{2} \| P_2 \|^2_{W^{1,2}(\Omega)} \tag{4.74}$$

$$+ \frac{1}{2\varepsilon_5} \| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}) \|^2_{L^2(\Omega)} + \frac{\varepsilon_5}{2} \| P_2 \|^2_{W^{1,2}(\Omega)} \Big)$$

for arbitrary ε_4, $\varepsilon_5 > 0$. With the choice $(\varepsilon_4 + \varepsilon_5) = 1/C$, we arrive at

$$\frac{1}{2} \| P_2(s) \|^2_{W^{1,2}(\Omega)} \leqslant C \Big(\| \nabla P_1 \|^2_{\left(W^{1,2}(\Omega)\right)^*} + \| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}) \|^2_{L^2(\Omega)} \Big) \quad \Longrightarrow \tag{4.75}$$

$$\| P_2 \|^2_{L^2\left[(0,T), W^{1,2}(\Omega)\right]} \leqslant 2C \Big(\| \nabla P_1 \|^2_{L^2\left[(0,T), \left(W^{1,2}(\Omega)\right)^*\right]} + \| \frac{\partial r}{\partial \eta}(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}) \|^2_{L^2(\Omega_T)} \Big) \tag{4.76}$$

where the right-hand side is bounded by Step 5.

• **Step 8.** *Conclusion of the proof.* The fact that P_1 belongs even to $C^0\big[[0,T], L^2(\Omega)\big]$ can be confirmed analogously to [Bourgault/Coudiére/Pierre 09], p. 478, Subsection 5.3. As a consequence of the imbedding theorem [Evans 98], p. 286, Theorem 2, $P_3 \in C^0\big[[0,T], L^2(\Omega)\big]$ holds true as well. Consequently, the norms on the left-hand side of (4.50) can be replaced by $C^0\big[[0,T], L^2(\Omega)\big]$-norms, and the proof is complete. ■

Remarks. 1) If the Rogers-McCulloch model in (3.12) – (3.14) is replaced by the FitzHugh-Nagumo model, the proofs of Theorems 4.1. and 4.2. can be repeated with only minor alterations.

2) Consider now (3.12) – (3.14) with the linearized Aliev-Panfilov model. Then, in the proof of Theorem 4.1., the first modification concerns (4.26), which must be replaced by

$$\hat{W}(x,t) = W_0(x)\, e^{-\varepsilon t} + \varepsilon\, \kappa \int_0^t \Big((a+1)\, \hat{\Phi}_{tr}(x,\tau) - \hat{\Phi}^2_{tr}(x,\tau) \Big)\, e^{\varepsilon(\tau - t)}\, d\tau, \tag{4.77}$$

thus belonging to $C^0\big[[0,T], L^3(\Omega)\big]$ only. Nevertheless, (4.40) remains true. Further, considering

$$\frac{\partial G}{\partial \varphi}(\hat{\Phi}_{tr}, \hat{W}) = -\varepsilon\, \kappa\, (a+1) + \varepsilon\, \kappa\, \hat{\Phi}_{tr}, \tag{4.78}$$

estimation (4.36) ff. has to be modified in the following way: On the right-hand side of (4.37), the term $\varepsilon\,\kappa\,\int_\Omega |\,P_1\,P_3\,|\,dx$ must be replaced by

$$\varepsilon\,\kappa\,(a+1)\int_\Omega |\,P_1\,P_3\,|\,dx\,+\,\varepsilon\,\kappa\int_\Omega |\,\hat{\Phi}_{tr}\,P_1\,P_3\,|\,dx\,. \tag{4.79}$$

The estimation of the first member of (4.79) runs as above; for the second one we get analogously to (4.44) ff. with arbitrary $\varepsilon_6>0$:

$$\int_\Omega |\,\hat{\Phi}_{tr}\,P_1\,P_3\,|\,dx\,\leqslant\,\frac{\varepsilon_6}{2}\int_\Omega |\hat{\Phi}_{tr}\,P_1\,|^2\,dx+\frac{1}{2\,\varepsilon_6}\,\|\,P_3\,\|^2_{L^2(\Omega)} \tag{4.80}$$

$$\leqslant\,\frac{\varepsilon_6}{2}\,\Big(\int_\Omega |\,\hat{\Phi}_{tr}\,|^4\,dx\Big)^{1/2}\Big(\int_\Omega |\,P_1\,|^4\,dx\Big)^{1/2}+\frac{1}{2\,\varepsilon_6}\,\|\,P_3\,\|^2_{L^2(\Omega)} \tag{4.81}$$

$$\leqslant\,C\,\Big(\,\frac{\varepsilon_6}{2}\,\|\,\hat{\Phi}_{tr}(s)\,\|^2_{W^{1,2}(\Omega)}\cdot\|\,P_1\,\|^2_{W^{1,2}(\Omega)}+\frac{1}{2\,\varepsilon_6}\,\|\,P_3\,\|^2_{L^2(\Omega)}\,\Big)\,, \tag{4.82}$$

and due to $\hat{\Phi}_{tr}\in L^\infty\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big]$, Steps 3 and 4 can be completed as before. A further alteration concerns the estimations (4.54) ff. in Step 5. In (4.56), the term $\sup_{\dots}\,\varepsilon^2\,\kappa^2\,\big(\int_\Omega |\,P_3\,|\,|\psi\,|\,dx\big)^2$ must be replaced by

$$\sup_{\dots}\,\varepsilon^2\,\kappa^2\,(a+1)^2\,\Big(\int_\Omega |\,P_3\,|\,|\psi\,|\,dx\Big)^2+\sup_{\dots}\,\varepsilon^2\,\kappa^2\,\Big(\int_\Omega |\,\hat{\Phi}_{tr}\,P_3\,\psi\,|\,dx\Big)^2\,, \tag{4.83}$$

providing the following estimate for the second member:

$$\sup_{\dots}\Big(\int_\Omega |\,\hat{\Phi}_{tr}\,P_3\,\psi\,|\,dx\Big)^2\,\leqslant\,C\,\sup_{\dots}\,\|\,P_3\,\|^2_{L^2(\Omega)}\cdot\|\,\hat{\Phi}_{tr}(s)\,\|^2_{L^3(\Omega)}\cdot\|\,\psi\,\|^2_{L^6(\Omega)}\,\leqslant\,C\,\|\,P_3\,\|^2_{L^2(\Omega)} \tag{4.84}$$

due again to the essential boundedness of the norms $\|\,\hat{\Phi}_{tr}(s)\,\|_{W^{1,2}(\Omega)}$ as well as to the imbedding $W^{1,2}(\Omega)\hookrightarrow L^6(\Omega)$. Then Step 5 can be finished as above, and the remaining parts of the proof remain unchanged.

Proof of Theorem 4.2. • Step 1. *Approximate solutions for the reduced system.* By [Bourgault/Coudiére/Pierre 09] , p. 464, Theorem 6, the bidomain bilinear form $A(\,\cdot\,,\,\cdot\,)$ gives rise to an orthonormal basis of eigenfunctions $\{\,\psi_i\,\}$ within the space $W^{1,2}(\Omega)$, which are related to eigenvalues $0=\lambda_0<\lambda_1\leqslant\lambda_2\leqslant\,\dots$. For $N\in\mathbb{N}_0$, let us define the subspaces

$$\mathrm{X}^N(\Omega)\,=\,\big\{\,\psi=\sum_{i=0}^N c_i\,\psi_i\;\big|\;c_0\,,\,\dots\,,\,c_N\in\mathbb{R}\,\big\}\subset W^{1,2}(\Omega)\,, \tag{4.85}$$

and the functions $P_1^N,\,P_3^N:\,\Omega\,\times[\,0\,,\,T\,]\to\mathrm{X}^N$ according to

$$P_1^N(x,s)\,=\,\sum_{i=0}^N p_{i,N}(s)\,\psi_i(x)\,;\quad P_3^N(x,s)\,=\,\sum_{i=0}^N q_{i,N}(s)\,\psi_i(x) \tag{4.86}$$

where $p_{i,N},\,q_{i,N}:\,[\,0\,,\,T\,]\to\mathbb{R}$ are solutions of the initial value problem

$$\frac{dp_{j,N}(s)}{ds}\,+\,\lambda_j\,p_{j,N}(s)+\sum_{i=0}^N p_{i,N}(s)\cdot\int_\Omega\frac{\partial I_{ion}}{\partial\varphi}(\hat{\Phi}_{tr},\hat{W})\,\psi_i(x)\,\psi_j(x)\,dx \tag{4.87}$$

$$+\sum_{i=0}^N q_{i,N}(s)\cdot\int_\Omega\frac{\partial G}{\partial\varphi}(\hat{\Phi}_{tr},\hat{W})\,\psi_i(x)\,\psi_j(x)\,dx\,=\,\langle\,\widetilde{S}(s)\,,\,\psi_j\,\rangle\,,\quad 0\leqslant j\leqslant N\,;$$

$$\frac{dq_{j,N}(s)}{ds}\,+\sum_{i=0}^N p_{i,N}(s)\cdot\int_\Omega\frac{\partial I_{ion}}{\partial w}(\hat{\Phi}_{tr},\hat{W})\,\psi_i(x)\,\psi_j(x)\,dx \tag{4.88}$$

$$+\sum_{i=0}^N q_{i,N}(s)\cdot\int_\Omega\frac{\partial G}{\partial w}(\hat{\Phi}_{tr},\hat{W})\,\psi_i(x)\,\psi_j(x)\,dx\,=\,-\langle\,\frac{\partial r}{\partial w}(\hat{\Phi}_{tr},\hat{\Phi}_e,\hat{W})\,,\,\psi_j\,\rangle\,,\quad 0\leqslant j\leqslant N\,;$$

$$p_{j,N}(0)\,=\,0\,;\;q_{j,N}(0)\,=\,0\quad 0\leqslant j\leqslant N\,. \tag{4.89}$$

Specifying the data for (4.87) $-$ (4.89) according to the Rogers-McCulloch model, the problem reads as

$$\frac{dp_{j,N}(s)}{ds} + \lambda_j\, p_{j,N}(s) + \sum_{i=0}^{N} p_{i,N}(s)\cdot \int_\Omega \Big(3\,b\,(\hat\Phi_{tr})^2 + 2\,(a+1)\,b\,\hat\Phi_{tr} + \hat W + a\,b \Big)\,\psi_i\,\psi_j\,dx \tag{4.90}$$
$$- \varepsilon\,\kappa\,q_{j,N}(s) = \langle\, \widetilde S(s)\,,\,\psi_j\,\rangle\,, \quad 0 \leqslant j \leqslant N\,;$$
$$\frac{dq_{j,N}(s)}{ds} + \sum_{i=0}^{N} p_{i,N}(s)\cdot \int_\Omega \hat\Phi_{tr}\,\psi_i\,\psi_j\,dx + \varepsilon\,q_{j,N}(s) = -\langle\, \frac{\partial r}{\partial w}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,,\,\psi_j\,\rangle\,, \quad 0 \leqslant j \leqslant N\,; \tag{4.91}$$
$$p_{j,N}(0) = 0\,;\ q_{j,N}(0) = 0 \quad 0 \leqslant j \leqslant N\,. \tag{4.92}$$

Obviously, all integrals with respect to x are well-defined and the coefficients as well as the right-hand sides are integrable with respect to s at least. Then, by [WARGA 72], p. 92, Theorem II.4.6., the initial-value problem (4.90) $-$ (4.92) admits a unique solution $\big(p_{0,N},\,\dots,\,p_{N,N}\,,\,q_{0,N}\,,\,\dots,\,q_{N,N}\big) \in \big(W^{1,1}(\,0\,,\,T\,)\big)^{2\,(N+1)}$. The same holds true if the Rogers-McCulloch model within (4.87) $-$ (4.89) is replaced by another model from Subsection 2.b). As a consequence of the orthogonality relations, P_1^N and P_3^N obey the equations

$$\frac{d}{ds}\langle\, P_1^N(s)\,,\,\psi\,\rangle + A\big(\,P_1^N(s)\,,\,\psi\,\big) + \int_\Omega \Big(\frac{\partial I_{ion}}{\partial\varphi}(\hat\Phi_{tr},\hat W)\,P_1^N + \frac{\partial G}{\partial\varphi}(\hat\Phi_{tr},\hat W)\,P_3^N \Big)\,\psi\,dx \tag{4.93}$$
$$= \langle\, \widetilde S(s)\,,\,\psi\,\rangle \quad \forall\,\psi \in \mathrm{X}^N(\Omega)\,;$$
$$\frac{d}{ds}\langle\, P_3^N(s)\,,\,\psi\,\rangle + \int_\Omega \Big(\frac{\partial I_{ion}}{\partial w}(\hat\Phi_{tr},\hat W)\,P_1^N + \frac{\partial G}{\partial w}(\hat\Phi_{tr},\hat W)\,P_3^N \Big)\,\psi\,dx \tag{4.94}$$
$$= -\langle\, \frac{\partial r}{\partial w}(\hat\Phi_{tr},\hat\Phi_e,\hat W)\,,\,\psi\,\rangle \quad \forall\,\psi \in \mathrm{X}^N(\Omega)\,.$$

In this sense, the functions P_1^N, P_3^N can be interpreted as approximate solutions of the reduced adjoint system.

• **Step 2.** *A-priori estimates for the approximate solutions* P_1^N, P_3^N. The functions P_1^N, P_3^N obey the a-priori estimates from Theorem 4.1. More precisely, the following holds:

Lemma 4.4. *Let the assumptions of Theorem 4.1. hold for the data of* (P) *and a feasible solution* $(\hat\Phi_{tr},\hat\Phi_e,\hat W,\hat I_e)$. *Then for all* $N \in \mathbb{N}_0$, *the functions* P_1^N, P_3^N *satisfy the estimate*

$$\|\,P_1^N\,\|^2_{C^0[\,[\,0\,,T\,]\,,\,L^2(\Omega)\,]} + \|\,P_1^N\,\|^4_{L^4[\,(\,0\,,T\,)\,,\,W^{1,2}(\Omega)\,]} + \|\,\partial P_1^N/\partial s\,\|^2_{L^2[\,(\,0\,,T\,)\,,\,(W^{1,2}(\Omega))^*\,]} \tag{4.95}$$
$$+ \|\,P_3^N\,\|^2_{C^0[\,[\,0\,,T\,]\,,\,L^2(\Omega)\,]} + \|\,\partial P_3^N/\partial s\,\|^2_{L^2(\Omega_T)} \leqslant C$$

for a constant $C > 0$ *independent of* N.

Proof. We rely on the proof of Theorem 4.1. First, we observe that (4.50) and (4.53) remain true if P_1 and P_3 are replaced by P_1^N and P_3^N since, in Steps $2-4$ of the proof above, the reduced equations must be studied only for the special test functions $P_1^N(s)$, $P_3^N(s) \in \mathrm{X}^N(\Omega)$. Lemma 4.3. carries over as well. Further, we observe that

$$\|\,\partial P_1^N/\partial s\,\|^2_{L^2[\,(\,0\,,T\,)\,,\,(W^{1,2}(\Omega))^*\,]} = \int_0^T \sup_{\|\,\psi\,\|_{W^{1,2}(\Omega)}\,=\,1} \big|\,\langle\,\partial P_1^N(s)/\partial s\,,\,\psi\,\rangle\,\big|^2\,ds \tag{4.96}$$
$$= \int_0^T \sup_{\|\,\sum_{j=0}^{\infty} c_j\,\psi_j\,\|_{W^{1,2}(\Omega)}\,=\,1} \big|\,\langle\,\sum_{i=0}^{N}\frac{dp_{i,N}(s)}{ds}\,\psi_i\,,\,\sum_{j=0}^{\infty} c_j\,\psi_j\,\rangle\,\big|^2\,ds \tag{4.97}$$

$$= \int_0^T \sup_{\| \sum_{j=0}^{\infty} c_j \psi_j \|_{W^{1,2}(\Omega)} = 1} \big| \langle \sum_{i=0}^{N} \frac{dp_{i,N}(s)}{ds} \psi_i \, , \, \sum_{j=0}^{N} c_j \psi_j \rangle \big|^2 \, ds \tag{4.98}$$

$$= \int_0^T \sup_{\psi \in \mathrm{X}^N \, , \, \| \psi \|_{W^{1,2}(\Omega)} = 1} \big| \langle \partial P_1^N(s)/\partial s \, , \, \psi \rangle \big|^2 \, ds \, . \tag{4.99}$$

By (4.93), the calculations from the proof of Theorem 4.1., Step 5, can be repeated now, resulting in a uniform bound for $\| \partial P_1^N/\partial s \|^2_{L^2 [(0,T), (W^{1,2}(\Omega))^*]}$. In the same manner, we may repeat the derivation from Step 6 since

$$\| \partial P_3^N/\partial s \|^2_{L^2 [(0,T), (L^2(\Omega))^*]} = \int_0^T \sup_{\| \psi \|_{L^2(\Omega)} = 1} \big| \langle \partial P_3^N(s)/\partial s \, , \, \psi \rangle \big|^2 \, ds \tag{4.100}$$

$$= \int_0^T \sup_{\psi \in \mathrm{X}^N \, , \, \| \psi \|_{L^2(\Omega)} = 1} \big| \langle \partial P_3^N(s)/\partial s \, , \, \psi \rangle \big|^2 \, ds \, , \tag{4.101}$$

and we obtain a uniform bound for $\| \partial P_3^N/\partial s \|^2_{L^2(\Omega_T)}$ as well. The arguments from Step 8 hold without alterations. If the Rogers-McCulloch model in (3.12) – (3.14) is replaced by another model from Subsection 2.b) then the corresponding modifications of the proof of Theorem 4.1. carry over to the proof of Lemma 4.4. as well. ∎

• **Step 3.** *An exact solution for the reduced adjoint system.* Lemma 4.4. implies that we may select a subsequence $\{ (P_1^{N'}, P_3^{N'}) \}$ of $\{ (P_1^N, P_3^N) \}$ with convergence to limit elements in the following sense:

$$P_1^{N'} \rightharpoonup^{L^4 [(0,T), W^{1,2}(\Omega)]} P_1 \, ; \tag{4.102}$$

$$dP_1^{N'}/ds \rightharpoonup^{L^2 [(0,T), (W^{1,2}(\Omega))^*]} \widetilde{P} \, ; \tag{4.103}$$

$$P_3^{N'} \rightharpoonup^{L^2 [(0,T), L^2(\Omega)]} P_3 \, ; \tag{4.104}$$

$$dP_3^{N'}/ds \rightharpoonup^{L^2 [(0,T), (L^2(\Omega))^*]} \widetilde{Q} \, . \tag{4.105}$$

Consequently, taking an arbitrary element $\psi_j \in W^{1,2}(\Omega)$ from the orthonormal base, we find

$$\begin{aligned} &\langle \widetilde{P}(s) \, , \, \psi_j \rangle + A\big(P_1(s) \, , \, \psi_j \big) + \int_\Omega \Big(\frac{\partial I_{ion}}{\partial \varphi}(\hat{\Phi}_{tr}, \hat{W}) \, P_1 + \frac{\partial G}{\partial \varphi}(\hat{\Phi}_{tr}, \hat{W}) \, P_3 \Big) \psi_j \, dx - \langle \widetilde{S}(s) \, , \, \psi_j \rangle \\ &\quad = \lim_{N' \to \infty} \Big(\frac{d}{ds} \langle P_1^{N'}(s) \, , \psi_j \rangle + A\big(P_1^{N'}(s) \, , \, \psi_j \big) + \int_\Omega \Big(\frac{\partial I_{ion}}{\partial \varphi}(\hat{\Phi}_{tr}, \hat{W}) \, P_1^{N'} \\ &\qquad + \frac{\partial G}{\partial \varphi}(\hat{\Phi}_{tr}, \hat{W}) \, P_3^{N'} \Big) \psi_j \, dx - \langle \widetilde{S}(s) \, , \, \psi_j \rangle \Big) = 0 \end{aligned} \tag{4.106}$$

since $\psi_j \in \mathrm{X}^{N'}$ for all sufficiently large $N' \in \mathbb{N}$. For the same reason, it holds that

$$\begin{aligned} &\langle \widetilde{Q}(s) \, , \, \psi_j \rangle + \int_\Omega \Big(\frac{\partial I_{ion}}{\partial w}(\hat{\Phi}_{tr}, \hat{W}) \, P_1 + \frac{\partial G}{\partial w}(\hat{\Phi}_{tr}, \hat{W}) \, P_3 \Big) \psi_j \, dx + \langle \frac{\partial r}{\partial w}(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}) \, , \, \psi_j \rangle \\ &\quad = \lim_{N' \to \infty} \Big(\frac{d}{ds} \langle P_3^{N'}(s) \, , \, \psi_j \rangle + \int_\Omega \Big(\frac{\partial I_{ion}}{\partial w}(\hat{\Phi}_{tr}, \hat{W}) \, P_1^{N'} + \frac{\partial G}{\partial w}(\hat{\Phi}_{tr}, \hat{W}) \, P_3^{N'} \Big) \psi_j \, dx \\ &\qquad + \langle \frac{\partial r}{\partial w}(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}) \, , \, \psi_j \rangle \Big) = 0 \, . \end{aligned} \tag{4.107}$$

Weak continuity of the distributional differential operator implies that $\widetilde{P} = dP_1/ds$ and $\widetilde{Q} = dP_3/ds$ in the sense of distributions. Further, it obviously holds that $P_1(x,0) = \lim_{N' \to \infty} P_1^N(x,0) = 0$ and $P_3(x,0) =$

$\lim_{N'\to\infty} P_3^N(x,0) = 0$. Since $\{\,\psi_i\,\}$ lies dense in $W^{1,2}(\Omega)$ as well as in $L^2(\Omega)$, the functions P_1 and P_3 form a weak solution of the reduced adjoint system.

• **Step 4.** *Completion of the adjoint solution.* As indicated in Subsection 4.b), the solution (P_1, P_3) of the reduced adjoint system may be completed to a weak solution (P_1, P_2, P_3) of the adjoint system where $P_2 \in L^2\big[\,(0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big]$ with $\int_\Omega P_2(x,s)\,dx = 0\ (\forall)\,s \in (\,0\,,\,T\,)$ is uniquely determined by P_1, P_3. This finishes the proof of Theorem 4.2. ■.

5. Necessary optimality conditions.

a) Statement of the theorems.

Definition 5.1. (Weak local minimizer) *A quadruple* $(\hat\Phi_{tr}, \hat\Phi_e, \hat W, \hat I_e)$*, which is feasible in* (P)*, is called a weak local minimizer of* (P) *iff there exists a number* $\varepsilon > 0$ *such that for all admissible* $(\Phi_{tr}, \Phi_e, W, I_e)$ *the conditions*

$$\|\,\Phi_{tr} - \hat\Phi_{tr}\,\|_{X_1} \leqslant \varepsilon\,,\ \ \|\,\Phi_e - \hat\Phi_e\,\|_{X_2} \leqslant \varepsilon\,,\ \ \|\,W - \hat W\,\|_{X_3} \leqslant \varepsilon\,,\ \ \|\,I_e - \hat I_e\,\|_{X_4} \leqslant \varepsilon \tag{5.1}$$

imply the relation $F(\hat\Phi_{tr}, \hat\Phi_e, \hat W, \hat I_e) \leqslant F(\Phi_{tr}, \Phi_e, W, I_e)$.

The necessary optimality conditions for weak local minimizers of (P) can be formulated as follows:

Theorem 5.2. (First-order necessary optimality conditions for the control problem (P)**)** *We study problem* (P) *under the assumptions of Subsection 3.a), specifying within* (3.12) − (3.14) *any of the three models from Subsection 2.b). Assume further that the integrand* $r(x,t,\varphi,\eta,w)$ *is continuously differentiable with respect to* φ*,* η *and* w*. If a quadruple* $(\hat\Phi_{tr}, \hat\Phi_e, \hat W, \hat I_e) \in L^2\big[\,(0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big] \times L^2\big[\,(0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big] \times L^2(\Omega_T) \times L^\infty\big[\,(0\,,\,T\,)\,,\,L^2(\Omega)\,\big]$ *is a weak local minimizer of* (P) *with*

$$\frac{\partial r}{\partial\varphi}(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\,,\ \frac{\partial r}{\partial\eta}(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\,,\ \frac{\partial r}{\partial w}(\hat\Phi_{tr}, \hat\Phi_e, \hat W) \in L^4\big[\,(0\,,\,T\,)\,,\,L^2(\Omega)\,\big] \tag{5.2}$$

then there exist multipliers $P_1 \in L^4\big[\,(0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big]$*,* $P_2 \in L^2\big[\,(0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big] \cap \big\{\,Z \mid \int_\Omega Z(x,t)\,dx = 0\ (\forall)\,t \in (\,0\,,\,T\,)\,\big\}$ *and* $P_3 \in L^2(\Omega_T)$*, satisfying together with* $(\hat\Phi_{tr}, \hat\Phi_e, \hat W, \hat I_e)$ *the adjoint equations* (4.8) − (4.10)*, which are solved in weak sense, as well as the optimality condition*

$$\int_0^T \int_{\Omega_{con}} \Big(\mu\,\hat I_e - Q\,P_2\Big) \cdot \big(\,I_e - \hat I_e\,\big)\,dx\,dt \geqslant 0 \quad \forall\,I_e \in \mathcal{C}\,. \tag{5.3}$$

Corollary 5.3. (Pointwise formulation of the optimality condition) *Under the assumptions of Theorem 5.2., let the optimal control* $\hat I_e$ *be represented as* $\hat I_e = Q\,\hat I$ *with* $\hat I \in L^\infty\big[\,(0\,,\,T\,)\,,\,L^2(\Omega)\,\big]$, $\operatorname{supp}(\hat I) \subseteq \Omega_{con} \times [\,0\,,\,T\,]$ *and* $|\,\hat I(x,t)\,| \leqslant R$ *for almost all* $(x,t) \in \Omega_T$*. The optimality condition* (5.3) *from Theorem 5.2. then implies the following Pontryagin minimum condition, which holds a. e. pointwise:*

$$\hat I(x_0,t_0) \cdot \Big(\,\mu \cdot Q\,\hat I(x_0,t_0) - Q\,P_2(x_0,t_0)\,\Big) = \underset{-R \leqslant \eta \leqslant R}{\mathrm{Min}}\ \eta\,\Big(\,\mu \cdot Q\,\hat I(x_0,t_0) - Q\,P_2(x_0,t_0)\,\Big) \tag{5.4}$$

$$(\forall)\,(x_0,t_0) \in \Omega_{con} \times [\,0\,,\,T\,]\,.$$

Consequently, for a. e. $(x,t) \in \Omega_{con} \times [\,0\,,\,T\,]$ *the following implications hold:*

$$\begin{aligned} &Q\,\hat I(x,t) - \frac{1}{\mu}\,Q\,P_2(x,t) > 0 \implies \hat I(x,t) = -R\,;\\ &Q\,\hat I(x,t) - \frac{1}{\mu}\,Q\,P_2(x,t) < 0 \implies \hat I(x,t) = \ \ R \ \text{ and}\\ &\hat I(x,t) \in (\,-R\,,\,R\,) \implies Q\,\hat I(x,t) - \frac{1}{\mu}\,Q\,P_2(x,t) = 0\,. \end{aligned} \tag{5.5}$$

Corollary 5.4. (Regularity of weak local minimizers) *Under the assumptions of Theorem 5.2., consider a weak local minimizer* $(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ *of* (P)*, whose control part* $\hat{I}_e = Q\,\hat{I}$ *is generated by a function* $\hat{I}$ *with* $|\,\hat{I}(x,t)\,| < R$ *a. e. Then* $\hat{I}_e\,\big|\,\Omega_{con}$ *belongs to the space* $L^\infty\big(\,\Omega_{con}\,\times\,[\,0\,,\,T\,]\,\big)\,\cap\,L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega_{con})\,\big]$.

Fur numerical purposes, it is useful to specify the Gâteaux derivative of the reduced cost functional $\widetilde{F}:\,\mathcal{C}\to\mathbb{R}$. It is defined through

$$\widetilde{F}(I_e)\;=\;F\big(\,\Phi_{tr}(I_e),\,\Phi_e(I_e),\,W(I_e),\,I_e\,\big) \tag{5.6}$$

with the aid of the control-to-state mapping $I_e\;\longmapsto\;\big(\,\Phi_{tr}(I_e),\,\Phi_e(I_e),\,W(I_e)\,\big)$, which is well-defined by Proposition 3.1.

Corollary 5.5. (First variation of the reduced cost functional) *Under the assumptions of Theorem 5.2., the Gâteaux derivative of the reduced cost functional* $\widetilde{F}$ *at* $\hat{I}_e\in\mathcal{C}$ *is given through*

$$D_{I_e}\widetilde{F}(\hat{I}_e)\;=\;\mu\,\hat{I}_e-Q\,P_2(\hat{I}_e) \tag{5.7}$$

where $\big(\,P_1(\hat{I}_e),\,P_2(\hat{I}_e),\,P_3(\hat{I}_e)\,\big)$ *denotes the solution of the adjoint system* (4.8) – (4.10) *corresponding to* $\big(\,\Phi_{tr}(\hat{I}_e),\,\Phi_e(\hat{I}_e),\,W(\hat{I}_e),\,\hat{I}_e\,\big)$.

b) Proof of the necessary optimality conditions.

Proof of Theorem 5.2. As mentioned in the introduction, the proof of the necessary optimality conditions for (P) is based on the stability estimate for the bidomain system (Theorem 2.4.) and the existence theorem for the adjoint system (Theorem 4.2.), which will be invoked in Steps 2 and 3 of the proof, respectively.

• **Step 1.** *Variation of the weak local minimizer in a feasible direction.* Assume that $(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ is a weak local minimizer of (P). If $I_e\in\mathcal{C}$ is an arbitrary feasible control with $\|\,I_e-\hat{I}_e\,\|_{L^\infty\left[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\,\right]}\leqslant\varepsilon$ then, by Proposition 3.2., all controls

$$I_e(s)\;=\;\hat{I}_e+s\,(I_e-\hat{I}_e)\,,\;\;0\leqslant s\leqslant 1\,, \tag{5.8}$$

belong to $\mathcal{C}$ as well. By Proposition 3.1., for every $I_e(s)\in L^\infty\big[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\,\big]$, there exists a corresponding weak solution $(\Phi_{tr}(s),\Phi_e(s),W(s))\in \mathrm{X}_1\times\mathrm{X}_2\times\mathrm{X}_3$ for the bidomain system on $[\,0\,,\,T\,]$. Thus the quadruples $(\Phi_{tr}(s),\Phi_e(s),W(s),I_e(s))$ are feasible in (P) for all $0\leqslant s\leqslant 1$. On the other hand, from [Kunisch/Wagner 11b], p. 7, Theorem 2.7. it follows that every feasible solution of (P) within a closed ball

$$\mathrm{U}_\varepsilon(\hat{\Phi}_{tr},\hat{\Phi}_e,\hat{W},\hat{I}_e)\;=\;\mathrm{K}(\hat{\Phi}_{tr},C\varepsilon)\,\times\,\mathrm{K}(\hat{\Phi}_e,C\varepsilon)\,\times\,\mathrm{K}(\hat{W},C\varepsilon)\,\times\,\mathrm{K}(\hat{I}_e,\varepsilon)\,\subset\,\mathrm{X}_1\times\mathrm{X}_2\times\mathrm{X}_3\times\mathrm{X}_4 \tag{5.9}$$

can be generated in this way.

• **Step 2. Lemma 5.6.** *For all* $I_e\in\mathcal{C}$, $\|\,I_e-\hat{I}_e\,\|_{L^\infty\left[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\,\right]}\leqslant\varepsilon$ *implies that*

$$\lim_{s\to 0+0}\frac{1}{s}\,\|\,\Phi_{tr}(s)-\hat{\Phi}_{tr}\,\|^2_{\mathrm{X}_1}\;=\;0\,;\qquad\lim_{s\to 0+0}\frac{1}{s}\,\|\,\Phi_{tr}(s)-\hat{\Phi}_{tr}\,\|^2_{\widetilde{\mathrm{X}}_1}\;=\;0\,; \tag{5.10}$$

$$\lim_{s\to 0+0}\frac{1}{s}\,\|\,\Phi_e(s)-\hat{\Phi}_e\,\|^2_{\mathrm{X}_2}\;=\;0\,; \tag{5.11}$$

$$\lim_{s\to 0+0}\frac{1}{s}\,\|\,W(s)-\hat{W}\,\|^2_{\mathrm{X}_3}\;=\;0\quad\textit{and}\quad\lim_{s\to 0+0}\frac{1}{s}\,\|\,W(s)-\hat{W}\,\|^2_{\widetilde{\mathrm{X}}_3}\;=\;0\,. \tag{5.12}$$

Proof. The stability estimate [Kunisch/Wagner 11b] p. 7, Theorem 2.7., (2.38), implies

$$\| \Phi_{tr}(s) - \hat\Phi_{tr} \|^2_{X_1} = \| \Phi_{tr}(s) - \hat\Phi_{tr} \|^2_{L^2[(0,T), W^{1,2}(\Omega)]} \leqslant C \cdot \| I_e(s) - \hat I_e \|^2_{L^\infty[(0,T), (W^{1,2}(\Omega))^*]}$$
$$\leqslant C \cdot \| I_e(s) - \hat I_e \|^2_{L^\infty[(0,T), L^2(\Omega)]} = C\, s^2 \, \| I_e - \hat I_e \|^2_{L^\infty[(0,T), L^2(\Omega)]} \implies \quad (5.13)$$
$$\lim_{s\to 0+0} \frac{1}{s} \| \Phi_{tr}(s) - \hat\Phi_{tr} \|^2_{X_1} \leqslant \lim_{s\to 0+0} C\, s \, \| I_e - \hat I_e \|^2_{L^\infty[(0,T), L^2(\Omega)]} = 0 \quad (5.14)$$

as well as

$$\| \Phi_e(s) - \hat\Phi_e \|^2_{X_2} = \| \Phi_e(s) - \hat\Phi_e \|^2_{L^2[(0,T), W^{1,2}(\Omega)]} \leqslant C \cdot \| I_e(s) - \hat I_e \|^2_{L^\infty[(0,T), (W^{1,2}(\Omega))^*]}$$
$$\leqslant C \cdot \| I_e(s) - \hat I_e \|^2_{L^\infty[(0,T), L^2(\Omega)]} = C\, s^2 \, \| I_e - \hat I_e \|^2_{L^\infty[(0,T), L^2(\Omega)]} \implies \quad (5.15)$$
$$\lim_{s\to 0+0} \frac{1}{s} \| \Phi_e(s) - \hat\Phi_e \|^2_{X_2} \leqslant \lim_{s\to 0+0} C\, s \, \| I_e - \hat I_e \|^2_{L^\infty[(0,T), L^2(\Omega)]} = 0 \quad (5.16)$$

and

$$\| W(s) - \hat W \|^2_{X_3} = \| W(s) - \hat W \|^2_{L^2(\Omega_T)} \leqslant C \cdot \| I_e(s) - \hat I_e \|^2_{L^\infty[(0,T), (W^{1,2}(\Omega))^*]}$$
$$\leqslant C \cdot \| I_e(s) - \hat I_e \|^2_{L^\infty[(0,T), L^2(\Omega)]} = C\, s^2 \, \| I_e - \hat I_e \|^2_{L^\infty[(0,T), L^2(\Omega)]} \implies \quad (5.17)$$
$$\lim_{s\to 0+0} \frac{1}{s} \| W(s) - \hat W \|^2_{X_3} \leqslant \lim_{s\to 0+0} C\, s \, \| I_e - \hat I_e \|^2_{L^\infty[(0,T), L^2(\Omega)]} = 0\,. \quad (5.18)$$

In an analogous manner, the relation with $\| W(s) - \hat W \|^2_{\widetilde{X}_3}$ can be confirmed. In order to establish the relation with $\| \Phi_{tr}(s) - \hat\Phi_{tr} \|^2_{\widetilde{X}_1}$, we rely on [Kunisch/Wagner 11b] p. 7, Theorem 2.7., (2.39), which leads to

$$\| \Phi_{tr}(s) - \hat\Phi_{tr} \|^2_{\widetilde{X}_1} = \| \Phi_{tr}(s) - \hat\Phi_{tr} \|^2_{W^{1,4/3}[(0,T), (W^{1,2}(\Omega))^*]} \quad (5.19)$$
$$\leqslant C^2 \cdot \mathrm{Max} \Big(\| I_e(s) - \hat I_e \|^2_{L^\infty[(0,T), (W^{1,2}(\Omega))^*]} \,,\, \| I_e(s) - \hat I_e \|^4_{L^\infty[(0,T), (W^{1,2}(\Omega))^*]} \Big) \quad (5.20)$$
$$\leqslant C \cdot \mathrm{Max} \Big(s^2 \, \| I_e - \hat I_e \|^2_{L^\infty[(0,T), L^2(\Omega)]} \,,\, s^4 \, \| I_e - \hat I_e \|^4_{L^\infty[(0,T), L^2(\Omega)]} \Big) \implies \quad (5.21)$$
$$\lim_{s\to 0+0} \frac{1}{s} \| \Phi_{tr}(s) - \hat\Phi_{tr} \|^2_{\widetilde{X}_1} \quad (5.22)$$
$$\leqslant \lim_{s\to 0+0} C \cdot \mathrm{Max} \Big(s \, \| I_e - \hat I_e \|^2_{L^\infty[(0,T), L^2(\Omega)]} \,,\, s^3 \, \| I_e - \hat I_e \|^4_{L^\infty[(0,T), L^2(\Omega)]} \Big) = 0\,. \quad \blacksquare$$

• **Step 3.** By Theorem 4.2., associated with $(\hat\Phi_{tr}, \hat\Phi_e, \hat W, \hat I_e)$, there exist functions $P_1 \in \big(L^{4/3}[(0,T), (W^{1,2}(\Omega))^*] \big)^* = L^4[(0,T), W^{1,2}(\Omega)]$, $P_2 \in \big(L^2[(0,T), W^{1,2}(\Omega)] \big)^* = L^2[(0,T), W^{1,2}(\Omega)]$ with $\int_\Omega P_2(x,t)\, dx = 0$ for almost all $t \in (0,T)$ and $P_3 \in \big(L^2[(0,T), (L^2(\Omega))^*] \big)^* = L^2(\Omega_T)$ satisfying the system (4.8) − (4.10) as weak solutions. Consequently, P_1, P_2 and P_3 solve the adjoint equations (4.5) − (4.7) together with $P_4 = -P_1(\,\cdot\,,0)$ and $P_5 = -P_3(\,\cdot\,,0)$. With these functions, we may derive the following estimates:

Lemma 5.7. *The following estimates hold true:*

$$\lim_{s\to 0+0} \frac{1}{s} \big\langle P_1 \,,\, D_{\Phi_{tr}} E_1(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\, (\Phi_{tr}(s) - \hat\Phi_{tr}) + D_{\Phi_e} E_1(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\, (\Phi_e(s) - \hat\Phi_e) \quad (5.23)$$
$$+ D_W E_1(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\, (W(s) - \hat W) \big\rangle = 0;$$
$$\lim_{s\to 0+0} \frac{1}{s} \big\langle P_2 \,,\, D_{\Phi_{tr}} E_2(\hat\Phi_{tr}, \hat\Phi_e, \hat I_e)\, (\Phi_{tr}(s) - \hat\Phi_{tr}) + D_{\Phi_e} E_2(\hat\Phi_{tr}, \hat\Phi_e, \hat I_e)\, (\Phi_e(s) - \hat\Phi_e) \quad (5.24)$$
$$+ \big\langle P_2 \,,\, D_{I_e} E_2(\hat\Phi_{tr}, \hat\Phi_e, \hat I_e)\, (I_e - \hat I_e) \big\rangle = 0;$$
$$\lim_{s\to 0+0} \frac{1}{s} \big\langle P_3 \,,\, D_{\Phi_{tr}} E_3(\hat\Phi_{tr}, \hat W)\, (\Phi_{tr}(s) - \hat\Phi_{tr}) + D_W E_3(\hat\Phi_{tr}, \hat W)\, (W(s) - \hat W) \big\rangle = 0\,. \quad (5.25)$$

Proof. We restrict ourselves to the proof of (5.23), noting that (5.24) and (5.25) can be confirmed in a completely analogous manner. Due to our assumptions on the differentiability of r, the principal theorem of calculus in its Bochner integral version [12] is applicable. For the feasible solutions $(\Phi_{tr}(s), \Phi_e(s), W(s), I_e(s))$ and $(\hat\Phi_{tr}, \hat\Phi_e, \hat W, \hat I_e)$, we get from the first state equation in (P), (3.12):

$$\begin{aligned}
\mathfrak{o} \;=\; & E_1(\Phi_{tr}(s), \Phi_e(s), W(s)) - E_1(\hat\Phi_{tr}, \hat\Phi_e, \hat W) \;=\; \int_0^1 D_{(\Phi_{tr},\Phi_e,W)}\, E_1\big(\,\hat\Phi_{tr} + \tau\,(\Phi_{tr}(s) - \hat\Phi_{tr})\,,\\
& \hat\Phi_e + \tau\,(\Phi_e(s) - \hat\Phi_e)\,,\, \hat W + \tau\,(W(s) - \hat W)\,\big)\,(\Phi_{tr}(s) - \hat\Phi_{tr}, \Phi_e(s) - \hat\Phi_e, W(s) - \hat W)\, d\tau \quad \Longrightarrow \qquad (5.26)\\
0 \;=\; & \Big\langle\, P_1\,,\, \int_0^1 \Big(D_{(\Phi_{tr},\Phi_e,W)}\, E_1\big(\,\hat\Phi_{tr} + \tau\,(\Phi_{tr}(s) - \hat\Phi_{tr})\,,\, \hat\Phi_e + \tau(\Phi_e(s) - \hat\Phi_e)\,,\, \hat W + \tau\,(W(s) - \hat W)\,\big)\\
& \qquad\qquad (\Phi_{tr}(s) - \hat\Phi_{tr}, \Phi_e(s) - \hat\Phi_e, W(s) - \hat W)\\
& - D_{(\Phi_{tr},\Phi_e,W)}\, E_1(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\,(\Phi_{tr}(s) - \hat\Phi_{tr}, \Phi_e(s) - \hat\Phi_e, W(s) - \hat W)\Big)\, d\tau\,\Big\rangle\\
& + \Big\langle\, P_1\,,\, D_{(\Phi_{tr},\Phi_e,W)}\, E_1(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\,(\Phi_{tr}(s) - \hat\Phi_{tr}, \Phi_e(s) - \hat\Phi_e, W(s) - \hat W)\,\Big\rangle \qquad (5.27)\\
=\; & \Big\langle\, P_1\,,\, \int_0^1 \Big(D_{\Phi_{tr}}\, E_1(\hat\Phi_{tr} + \tau \ldots, \hat\Phi_e + \tau \ldots, \hat W + \tau \ldots)\,(\Phi_{tr}(s) - \hat\Phi_{tr}) - D_{\Phi_{tr}}\, E_1(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\,(\Phi_{tr}(s) - \hat\Phi_{tr})\\
& + D_{\Phi_e}\, E_1(\hat\Phi_{tr} + \tau \ldots, \hat\Phi_e + \tau \ldots, \hat W + \tau \ldots)\,(\Phi_e(s) - \hat\Phi_e) - D_{\Phi_e}\, E_1(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\,(\Phi_e(s) - \hat\Phi_e) \qquad (5.28)\\
& + D_W\, E_1(\hat\Phi_{tr} + \tau \ldots, \hat\Phi_e + \tau \ldots, \hat W + \tau \ldots)\,(W(s) - \hat W) - D_W\, E_1(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\,(W(s) - \hat W)\Big)\, d\tau\,\Big\rangle\\
& + \Big\langle\, P_1\,,\, D_{\Phi_{tr}}\, E_1(\hat\Phi_{tr}, \hat\Phi_e, \hat W)(\Phi_{tr}(s) - \hat\Phi_{tr}) + D_{\Phi_e}\, E_1(\hat\Phi_{tr}, \hat\Phi_e, \hat W)(\Phi_e(s) - \hat\Phi_e)\\
& \qquad\qquad + D_W\, E_1(\hat\Phi_{tr}, \hat\Phi_e, \hat W)(W(s) - \hat W)\,\Big\rangle\,.
\end{aligned}$$

By [YOSIDA 95], p. 133, Corollary 1, we have

$$\Big|\,\Big\langle\, P_1\,,\, \int_0^1 (\,\ldots\,)\, d\tau\,\Big\rangle\,\Big| \;\leqslant\; \|\, P_1\,\|_{Z_1^*} \cdot \Big\|\, \int_0^1 (\,\ldots\,)\, d\tau\,\Big\|_{Z_1} \;\leqslant\; \|\, P_1\,\|_{Z_1^*} \cdot \int_0^1 \|\,\ldots\,\|_{Z_1}\, d\tau\,. \qquad (5.29)$$

Consequently, for the first summand within (5.28), it holds that

$$\begin{aligned}
& \lim_{s\to 0+0} \frac{1}{s}\,\Big|\,\Big\langle\, P_1\,,\, \int_0^1 (\,\ldots\,)\, d\tau\,\Big\rangle\,\Big| \;\leqslant\; \lim_{s\to 0+0} \|\, P_1\,\|_{Z_1^*} \Big(\int_0^1 |\, D_{\Phi_{tr}}\, E_1(\hat\Phi_{tr} + \tau \ldots, \hat\Phi_e + \tau \ldots, \hat W + \tau \ldots) \qquad (5.30)\\
& \qquad - D_{\Phi_{tr}}\, E_1(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\,\|_{\mathcal{L}(\widetilde{X}_1, Z_1)}\, \frac{1}{s}\, \|\, \Phi_{tr}(s) - \hat\Phi_{tr}\,\|_{\widetilde{X}_1}\, d\tau\\
& + \int_0^1 \big\|\, D_{\Phi_e}\, E_1(\hat\Phi_{tr} + \tau \ldots, \hat\Phi_e + \tau \ldots, \hat W + \tau \ldots,) - D_{\Phi_e}\, E_1(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\,\big\|_{\mathcal{L}(X_2, Z_1)}\, \frac{1}{s}\, \|\, \Phi_e(s) - \hat\Phi_e\,\|_{X_2}\, d\tau\\
& + \int_0^1 \big\|\, D_W\, E_1(\hat\Phi_{tr} + \tau \ldots, \hat\Phi_e + \tau \ldots, \hat W + \tau \ldots,) - D_W\, E_1(\hat\Phi_{tr}, \hat\Phi_e, \hat W)\,\big\|_{\mathcal{L}(\widetilde{X}_3, Z_1)}\, \frac{1}{s}\, \|\, W(s) - \hat W\,\|_{\widetilde{X}_3}\, d\tau\\
& \leqslant \lim_{s\to 0+0} \|\, P_1\,\|_{Z_1^*} \Big(\int_0^1 L_1\, \tau\, \Big(\, \|\, \Phi_{tr}(s) - \hat\Phi_{tr}\,\|_{\widetilde{X}_1} + \|\, \Phi_e(s) - \hat\Phi_e\,\|_{X_2} + \|\, W(s) - \hat W\,\|_{\widetilde{X}_3}\,\Big)\, \frac{1}{s}\, \|\, \Phi_{tr}(s) - \hat\Phi_{tr}\,\|_{\widetilde{X}_1}\, d\tau\\
& + \int_0^1 L_2\, \tau\, \Big(\int_0^1 L_1\, \tau\, \Big(\, \|\, \Phi_{tr}(s) - \hat\Phi_{tr}\,\|_{\widetilde{X}_1} + \|\, \Phi_e(s) - \hat\Phi_e\,\|_{X_2} + \|\, W(s) - \hat W\,\|_{\widetilde{X}_3}\,\Big)\, \frac{1}{s}\, \|\, \Phi_e(s) - \hat\Phi_e\,\|_{X_2}\, d\tau\\
& + \int_0^1 L_3\, \tau\, \Big(\|\, \Phi_{tr}(s) - \hat\Phi_{tr}\,\|_{\widetilde{X}_1} + \|\, \Phi_e(s) - \hat\Phi_e\,\|_{X_2} + \|\, W(s) - \hat W\,\|_{\widetilde{X}_3}\,\Big)\, \frac{1}{s}\, \|\, W(s) - \hat W\,\|_{\widetilde{X}_3}\, d\tau \qquad (5.31)
\end{aligned}$$

with Lipschitz constants L_1, L_2, L_3, whose existence is ensured by the twice continuous Fréchet differentiability of E_1 with respect to Φ_{tr}, Φ_e and W. With reference to Lemma 5.6., the estimate (5.31) may be

[12] [BERGER 77] , p. 68, (2.1.11).

continued as follows:

$$\lim_{s\to 0+0} \frac{1}{s} \,|\, \big\langle\, P_1 \,,\, \int_0^1 \big(\, ... \,\big)\, d\tau \,\big\rangle \,|$$

$$\leqslant \lim_{s\to 0+0} \|\, P_1 \,\|_{Z_1^*} \frac{1}{2} \big(\, L_1 + L_2 + L_3 \,\big)\, \frac{1}{s} \Big(\|\, \Phi_{tr}(s) - \hat{\Phi}_{tr} \,\|_{\widetilde{X}_1} + \|\, \Phi_e(s) - \hat{\Phi}_e \,\|_{X_2} + \|\, W(s) - \hat{W} \,\|_{\widetilde{X}_3} \Big)^2 \tag{5.32}$$

$$\leqslant \lim_{s\to 0+0} \|\, P_1 \,\|_{Z_1^*}\, C \,\Big(\frac{1}{s} \,\|\, \Phi_{tr}(s) - \hat{\Phi}_{tr} \,\|^2_{\widetilde{X}_1} + \frac{1}{s} \,\|\, \Phi_e(s) - \hat{\Phi}_e \,\|^2_{X_2} + \frac{1}{s} \,\|\, W(s) - \hat{W} \,\|^2_{\widetilde{X}_3} \Big) \,=\, 0 \,, \tag{5.33}$$

and this implies the first of the claimed relations, namely

$$\lim_{s\to 0+0} \frac{1}{s} \,\big\langle\, P_1 \,,\, D_{\Phi_{tr}}\, E_1(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W})\, (\Phi_{tr}(s) - \hat{\Phi}_{tr}) + D_{\Phi_e}\, E_1(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W})\, (\Phi_e(s) - \hat{\Phi}_e) \tag{5.34}$$

$$+ D_W\, E_1(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W})\, (W(s) - \hat{W}) \,\big\rangle \,=\, 0 \,.$$

From the second and third state equations (3.13) and (3.14), the limit relations (5.24) and (5.25) can be derived in a completely analogous way. ■

Since $\Phi_{tr}(s)$ and $W(s)$ take the same initial values as $\hat{\Phi}_{tr}$ and $\hat{W}$, respectively, it holds further that

$$\lim_{s\to 0+0} \frac{1}{s} \,\big\langle\, P_4 \,,\, D_{\Phi_{tr}}\, E_4(\hat{\Phi}_{tr})\, (\Phi_{tr}(s) - \hat{\Phi}_{tr}) \,\big\rangle \,=\, \lim_{s\to 0+0} \frac{1}{s} \,\big\langle\, P_5 \,,\, D_W\, E_5(\hat{W})\, (W(s) - \hat{W}) \,\big\rangle \,=\, 0 \,. \tag{5.35}$$

• **Step 4.** *The first variation of the objective.* Choose now $\varepsilon > 0$ small enough in order to ensure that the difference $F(\Phi_{tr}(s), \Phi_e(s), W(s), I_e(s)) - F(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ of the objective values is nonnegative for all quadruples $(\Phi_{tr}(s), \Phi_e(s), W(s), I_e(s))$ belonging to the closed ball $U_\varepsilon(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)$ defined in (5.9). As a consequence of our assumptions about the integrand r, the first variation may be written as

$$0 \,\leqslant\, \delta^+ F(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)\, (\Phi_{tr}(1) - \hat{\Phi}_{tr}, \Phi_e(1) - \hat{\Phi}_e, W(1) - \hat{W}, I_e - \hat{I}_e)$$

$$= \lim_{s\to 0+0} \frac{1}{s} \Big(F(\Phi_{tr}(s), \Phi_e(s), W(s), I_e(s)) - F(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e) \Big) \tag{5.36}$$

$$= \lim_{s\to 0+0} \frac{1}{s} \Big(D_{\Phi_{tr}}\, F(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)\, (\Phi_{tr}(s) - \hat{\Phi}_{tr}) + D_{\Phi_e}\, F(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)\, (\Phi_e(s) - \hat{\Phi}_e) \tag{5.37}$$

$$+ D_W\, F(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)\, (W(s) - \hat{W}) + D_{I_e}\, F(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)\, (I_e(s) - \hat{I}_e) \Big) \,.$$

Together with Lemma 5.7. and (5.35), we obtain

$$0 \,\leqslant\, \lim_{s\to 0+0} \frac{1}{s} \Big(D_{\Phi_{tr}}\, F(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)\, (\Phi_{tr}(s) - \hat{\Phi}_{tr}) \tag{5.38}$$

$$+ \big\langle\, P_1 \,,\, D_{\Phi_{tr}}\, E_1(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W})\, (\Phi_{tr}(s) - \hat{\Phi}_{tr}) \,\big\rangle + \big\langle\, P_2 \,,\, D_{\Phi_{tr}}\, E_2(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{I}_e)\, (\Phi_{tr}(s) - \hat{\Phi}_{tr}) \,\big\rangle$$

$$+ \big\langle\, P_3 \,,\, D_{\Phi_{tr}}\, E_3(\hat{\Phi}_{tr}, \hat{W})\, (\Phi_{tr}(s) - \hat{\Phi}_{tr}) \,\big\rangle + \big\langle\, P_4 \,,\, D_{\Phi_{tr}}\, E_4(\hat{\Phi}_{tr})\, (\Phi_{tr}(s) - \hat{\Phi}_{tr}) \,\big\rangle$$

$$+\, D_{\Phi_e}\, F(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)\, (\Phi_e(s) - \hat{\Phi}_e)$$

$$+ \big\langle\, P_1 \,,\, D_{\Phi_e}\, E_1(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W})\, (\Phi_e(s) - \hat{\Phi}_e) \,\big\rangle + \big\langle\, P_2 \,,\, D_{\Phi_e}\, E_2(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{I}_e)\, (\Phi_e(s) - \hat{\Phi}_e) \,\big\rangle$$

$$+ D_W\, F(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)\, (W(s) - \hat{W})$$

$$+ \big\langle\, P_1 \,,\, D_W\, E_1(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W})\, (W(s) - \hat{W}) \,\big\rangle + \big\langle\, P_2 \,,\, D_W\, E_2(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{I}_e)\, (W(s) - \hat{W}) \,\big\rangle$$

$$+ \big\langle\, P_3 \,,\, D_W\, E_3(\hat{\Phi}_{tr}, \hat{W})\, (W(s) - \hat{W}) \,\big\rangle + \big\langle\, P_5 \,,\, D_W\, E_5(\hat{W})\, (W(s) - \hat{W}) \,\big\rangle$$

$$+\, D_{I_e}\, F(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)\, (I_e(s) - \hat{I}_e) + \big\langle\, P_2 \,,\, D_{I_e}\, E_2(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{I}_e)\, (I_e - \hat{I}_e) \,\big\rangle \Big)$$

where the first three parts vanish since P_1, P_2, P_3 together with $P_4 = -P_1(\,\cdot\,,0)$ and $P_5 = -P_3(\,\cdot\,,0)$ solve the adjoint equations (4.5) – (4.7). Note that, by Subsection 4.a) above, these equations take the claimed form. Consequently, we arrive at

$$0 \leqslant \lim_{s\to 0+0} \frac{1}{s} \Big(D_{I_e}\, F(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{W}, \hat{I}_e)\,(I_e(s) - \hat{I}_e) + \big\langle\, P_2\,,\, D_{I_e}\, E_2(\hat{\Phi}_{tr}, \hat{\Phi}_e, \hat{I}_e)\,(I_e - \hat{I}_e)\,\big\rangle \Big) \tag{5.39}$$

$$= \int_0^T \int_\Omega \Big(\mu\, \hat{I}_e - P_2 \Big) \cdot \big(\, I_e - \hat{I}_e \,\big)\, dx\, dt \;=\; \int_0^T \int_\Omega \Big(\mu\, \hat{I}_e - Q\, P_2 \Big) \cdot \big(\, I_e - \hat{I}_e \,\big)\, dx\, dt \tag{5.40}$$

for arbitrary $I_e \in \mathcal{C}$. Since I_e and $\hat{I}_e$ vanish outside $\Omega_{con} \times [\,0\,,\,T\,]$, this confirms the claimed optimality condition (5.3), and the proof is complete. ■

Proof of Corollary 5.3. Using the representations $I_e = Q\,I$ and $\hat{I}_e = Q\,\hat{I}$, inequality (5.40) may be rewritten as

$$0 \leqslant \int_0^T \int_\Omega \Big(\mu \cdot Q\,\hat{I} - Q\,P_2 \Big) \cdot \big(\, Q\,I - Q\,\hat{I} \,\big)\, dx\, dt \;=\; \int_0^T \int_\Omega \Big(\mu \cdot Q\,\hat{I} - Q\,P_2 \Big) \cdot \big(\, I - \hat{I} \,\big)\, dx\, dt \tag{5.41}$$

$$= \int_0^T \int_{\Omega_{con}} \Big(\mu \cdot Q\,\hat{I} - Q\,P_2 \Big) \cdot \big(\, I - \hat{I} \,\big)\, dx\, dt \tag{5.42}$$

$$\forall\, I \in L^\infty\big[\,(\,0\,,\,T\,)\,,\,L^2(\Omega)\,\big] \;\; \textit{with} \;\; \operatorname{supp}(I) \subseteq \Omega_{con} \times [\,0\,,\,T\,] \;\; \textit{and} \;\; |\,I(x,t)\,| \leqslant R \;\; (\forall)\,(x,t) \in \Omega_T\,.$$

To (5.42), we may apply a Lebesgue point argument analogous to [Kunisch/Wagner 11a], p. 19 f., Proof of Corollary 3.6., in order to get

$$\Big(\mu \cdot Q\,\hat{I}(x_0,t_0) - Q\,P_2(x_0,t_0) \Big) \cdot \big(\, \eta_0 - \hat{I}(x_0,t_0) \,\big) \geqslant 0 \;\; \forall\, \eta_0 \in [\,-R\,,\,R\,] \;\; (\forall)\,(x_0,t_0) \in \Omega_{con} \times [\,0\,,\,T\,]\,, \tag{5.43}$$

and this implies the conditions (5.4) and (5.5). ■

Proof of Corollary 5.4. This is implied by (5.5) since $Q\,P_2\,\big|\,\Omega_{con} \in L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega_{con})\,\big]$ together with $P_2 \in L^2\big[\,(\,0\,,\,T\,)\,,\,W^{1,2}(\Omega)\,\big]$. ■

Proof of Corollary 5.5. We can follow the proof of Theorem 5.2. where only in (5.36), (5.38) and (5.39) the minorization by 0 must be deleted. ■

Acknowledgement.

The present work has been supported within the Special Research Unit "Mathematical Optimization and Applications in Biomedical Sciences" (Graz) by the Austrian Science Fund.

References.

1. [Ainseba/Bendamahne/Ruiz-Baier 10] Ainseba, B.; Bendamahne, M.; Ruiz-Baier, R.: *Analysis of an optimal control problem for the tridomain model in cardiac electrophysiology.* EPF Lausanne 2010; EPFL-REPORT-155519, 20 pp.
2. [Aliev/Panfilov 96] Aliev, R. R.; Panfilov, A. V.: *A simple two-variable model of cardiac excitation.* Chaos, Solitons & Fractals **7** (1996), 293 – 301
3. [Berger 77] Berger, M. S.: *Nonlinearity and Functional Analysis.* Academic Press; New York - San Francisco - London 1977
4. [Bourgault/Coudière/Pierre 09] Bourgault, Y.; Coudière, Y.; Pierre, C.: *Existence and uniqueness of the solution for the bidomain model used in cardiac electrophysiology.* Nonlinear Analysis: Real World Appl. **10** (2009), 458 – 482
5. [Brandão/Fernández-Cara/Magalhães/Rojas-Medar 08] Brandaõ, A. J. V.; Fernández-Cara, E.; Magalhães, P. M. D.; Rojas-Medar, M. A.: *Theoretical analysis and control results for the FitzHugh-Nagumo equation.* Electronic J. of Differential Equations, Vol. 2008, No. 164, 1 – 20 (electronically published)
6. [Dacorogna 08] Dacorogna, B.: *Direct Methods in the Calculus of Variations.* Springer; New York etc. 2008, 2nd ed.
7. [Evans 98] Evans, L. C.: *Partial Differential Equations.* American Mathematical Society; Providence 1998
8. [FitzHugh 61] FitzHugh, R.: *Impulses and physiological states in theoretical models of nerve membrane.* Biophysical J. **1** (1961), 445 – 466
9. [Ito/Kunisch 08] Ito, K.; Kunisch, K.: *Lagrange Multiplier Approach to Variational Problems and Applications.* SIAM; Philadelphia 2008
10. [Kunisch/Nagaiah/Wagner 11] Kunisch, K.; Nagaiah, C.; Wagner, M.: *A parallel Newton-Krylov method for optimal control of the monodomain model in cardiac electrophysiology.* University of Graz, Institute for Mathematics and Scientific Computing, SFB-Report No. 2011–005
11. [Kunisch/Wagner 11a] Kunisch, K.; Wagner, M.: *Optimal control of the bidomain system (I): The monodomain approximation with the Rogers-McCulloch model. Revised version.* University of Leipzig, Institute of Mathematics, Preprint No. 03/2011
12. [Kunisch/Wagner 11b] Kunisch, K.; Wagner, M.: *Optimal control of the bidomain system (II): Uniqueness and regularity theorems.* University of Graz, Institute for Mathematics and Scientific Computing, SFB-Report No. 2011–008
13. [Muzdeka/Barbieri 05] Muzdeka, S.; Barbieri, E.: *Control theory inspired considerations for the mathematical model defibrillation.* In: Proceedings of the 44th IEEE Conference on Decision and Control, 2005 and 2005 European Control Conference, 7416 – 7421
14. [Nagaiah/Kunisch 11] Nagaiah, C.; Kunisch, K.: *Higher order optimization and adaptive numerical solution for optimal control of monodomain equations in cardiac electrophysiology.* Appl. Num. Math. **61** (2011), 53 – 65
15. [Nagaiah/Kunisch/Plank 11] Nagaiah, C.; Kunisch, K.; Plank, G.: *Numerical solution for optimal control of the reaction-diffusion equations in cardiac electrophysiology.* Comput. Optim. Appl. **49** (2011), 149 – 178
16. [Nagumo/Arimoto/Yoshizawa 62] Nagumo, J.; Arimoto, S.; Yoshizawa, S.: *An active pulse transmission line simulating nerve axon.* Proceedings of the Institute of Radio Engineers **50** (1962), 2061 – 2070
17. [Rogers/McCulloch 94] Rogers, J. M.; McCulloch, A. D.: *A collocation-Galerkin finite element model of cardiac action potential propagation.* IEEE Transactions of Biomedical Engineering **41** (1994), 743 – 757
18. [Rolewicz 76] Rolewicz, S.: *Funktionalanalysis und Steuerungstheorie.* Springer; Berlin - Heidelberg - New York 1976

19. [SUNDNES/LINES/CAI/NIELSEN/MARDAL/TVEITO 06] Sundnes, J.; Lines, G. T.; Cai, X.; Nielsen, B. F.; Mardal, K.-A.; Tveito, A.: *Computing the Electrical Activity in the Heart.* Springer; Berlin etc. 2006
20. [TUNG 78] Tung, L.: *A Bi-Domain Model for Describing Ischemic Myocardial D-C Potentials.* PhD thesis. Massachusetts Institute of Technology 1978
21. [WARGA 72] Warga, J.: *Optimal Control of Differential and Functional Equations.* Academic Press; New York - London 1972
22. [YOSIDA 95] Yosida, K.: *Functional Analysis.* Springer; Berlin etc. 1995 (reprint of the 6th ed. from 1980)

Last modification: 14. 12. 2011

Authors' addresses / e-mail. *Karl Kunisch:* University of Graz, Institute for Mathematics and Scientific Computing, Heinrichstraße 36, A-8010 Graz, Austria. e-mail: `karl.kunisch@uni-graz.at`

Marcus Wagner: University of Leipzig, Department of Mathematics, P. O. B. 10 09 20, D-04009 Leipzig, Germany. Homepage / e-mail: `www.thecitytocome.de` / `marcus.wagner@math.uni-leipzig.de`