

A HOMOCLINIC SOLUTION FOR EXCITATION WAVES ON A CONTRACTILE SUBSTRATUM

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ABSTRACT. We analyze a model of electric signalling in biological tissues and prove that this model admits a travelling wave solution. Our result is based on a new technique for computing rigorous bounds on the stable and unstable manifolds at an equilibrium point of a dynamical system depending on a parameter.

1. MODELING, MOTIVATIONS AND MAIN RESULT

The mathematical modelling of electric signalling in biological tissues, and in the cardiac muscle in particular, is a longstanding problem that has attracted a number of efforts. The mathematical structure of a typical model consists of one reaction–diffusion equation, linear in the diffusion and nonlinear in the reaction term, coupled with one or more ordinary differential equations [9]. The classical model that incorporates this basic mathematical structure, while introducing the minimum amount of algebraic complications is given by the Fitzhugh–Nagumo equations:

$$(1.1) \quad \frac{\partial v}{\partial t} - \nabla \cdot (\mathbf{D}\nabla v) = -Av(v - \alpha)(v - 1) - Aw,$$

$$(1.2) \quad \frac{\partial w}{\partial t} = v - \frac{w}{\tau},$$

where $v(\mathbf{X}, t)$ is the action potential and $w(\mathbf{X}, t)$ is the gate variable. In general \mathbf{D} is a symmetric positive definite tensor and $A \simeq \|\mathbf{D}\| \gg 1$, where $\|\cdot\|$ denotes some suitable norm.

Recent papers [7, 11] have pointed out the role of the contractility of the substratum in real physiological conditions, where the electrical potential actually modulates the contraction of the muscle fibers and consequently the strain of the material. Equations (1.1,1.2) are therefore to be rewritten in moving coordinates, where the strain of the domain is driven by the action potential itself. It is convenient to rewrite the equations in material coordinates, using a mapping between current

positions and reference ones. Adopting the standard terminology of continuum mechanics, we denote by $\mathbf{x} = \mathbf{x}(\mathbf{X}, t)$ the position at time t of the material point that was at time $t = 0$ at \mathbf{X} . The gradient of deformation is therefore $\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}$ and the eqs. (1.1) and (1.2) rewritten on a contractile substratum in material coordinates read [7, 11],

$$(1.3) \quad \frac{\partial}{\partial t}(Jv) - \text{Div} (J\mathbf{F}^{-1}\mathbf{D}\mathbf{F}^{-T}\text{Grad} v) = -AJv(v - \alpha)(v - 1) - AJw,$$

$$(1.4) \quad \frac{\partial}{\partial t}(Jw) = Jv - \frac{Jw}{\tau},$$

where $J = \det(\mathbf{F})$ and the symbols Div and Grad denote operators with respect to \mathbf{X} .

Our goal in this paper is a rigorous, computer assisted, analysis of the one dimensional counterpart of eqs. (1.3) and (1.4)

$$(1.5) \quad \frac{\partial}{\partial t}(Jv) - \frac{\partial}{\partial X} D \left(J^{-1} \frac{\partial v}{\partial X} \right) = -AJv(v - \alpha)(v - 1) - AJw,$$

$$(1.6) \quad \frac{\partial}{\partial t}(Jw) = Jv - \frac{Jw}{\tau},$$

where the (scalar) diffusion coefficient D is taken constant and $J = \partial x / \partial X$. To make the problem well defined, we need to introduce a relation between the contraction of the substrate and the action potential. While this relation in real biological tissues is quite complicated, we choose the simple linear relation

$$(1.7) \quad \frac{\partial x}{\partial X} = 1 - \beta v,$$

where $\beta \in (0, 1)$ is a constant. The end result is [2]

$$(1.8) \quad \varepsilon \frac{\partial}{\partial t} ((1 - \beta v)v) - \frac{\partial}{\partial X} \left(\frac{1}{1 - \beta v} \frac{\partial v}{\partial X} \right) = -(1 - \beta v)v(v - \alpha)(v - 1) - (1 - \beta v)w,$$

$$(1.9) \quad \frac{\partial}{\partial t} ((1 - \beta v)w) = (1 - \beta v) \left(v - \frac{w}{\tau} \right).$$

where we have taken $A = D = \varepsilon^{-1}$.

In [2] it was found that eqs. (1.8) and (1.9), admit travelling pulse solutions that travel faster than in the rigid case. Our aim here is to give a proof for the existence of such a solution. To be more specific, we are interested in solutions of eqs. (1.8) and (1.9) of travelling wave type and finite energy, that is, solutions $v(t, X) = V(X - ct)$, $w(t, X) = W(X - ct)$, where V and W are homoclinic to 0. The system becomes

$$(1.10) \quad \begin{cases} \frac{V''}{1 - \beta V} = -\varepsilon c(1 - 2\beta V)V' - \frac{\beta(V')^2}{(1 - \beta V)^2} \\ \quad + (1 - \beta V)V(V - \alpha)(V - 1) + (1 - \beta V)W \\ W' = \frac{W}{c\tau} - \frac{V}{c} + \frac{\beta WV'}{1 - \beta V}, \end{cases}$$

Theorem 1. *Let $\alpha = 0.1$, $\beta = 0.3$, $\varepsilon = 0.01$, $\tau = 0.2$. There exists $c \in [c_0 - \delta, c_0 + \delta]$, with $c_0 = \frac{661961516}{11186863} \approx 59$ and $\delta = 2^{-43}$, such that the system (1.10) admits a solution homoclinic to 0.*

The proof of Theorem 1 is divided into several parts. In Section 2 we describe a general method to compute bounds on the invariant manifolds of nonlinear dynamical systems. This method is then applied to the system (1.10) as described in Section 3. It reduces the problem to a number of specific estimates that can be carried out with the aid of a computer. These estimates are described in the first part of Section 4. In the second part we discuss some of the details of our computer-assisted proof.

2. A PARAMETRIZATION FOR THE INVARIANT MANIFOLDS

Consider the nonlinear dynamical system in \mathbb{R}^N

$$(2.1) \quad y' = Ay + B(y),$$

for a curve $y : \mathbb{R} \rightarrow D$, where D is some open domain in \mathbb{R}^N containing the origin, A is an invertible linear map on \mathbb{R}^N , $B : D^* \rightarrow \mathbb{C}^N$ (where D^* is some open domain in \mathbb{C}^N that includes the closure of D) is analytic, $B(x) \in \mathbb{R}^N$ if $x \in D$ and $B(y) = O(|y|^2)$. By definition, the unstable manifold at 0 is the set of all initial conditions $y(0)$ such that $\lim_{t \rightarrow -\infty} y(t) = 0$. In the following, with no loss of generality, we will only consider the unstable manifold, since the stable manifold of (2.1) is the unstable manifold of $\dot{y} = -(Ay + B(y))$. It is well known that, under these assumptions, the unstable manifold is tangent in 0 to the eigenspace of A corresponding to eigenvalues with positive real part. We are interested in computing a parametrization of the local unstable manifold in a neighborhood of the origin, with rigorous bounds on the error. This problem was addressed in [8], where an explicit algorithm was introduced in the case where the matrix A only has real eigenvalues. Here we extend the approach to the generic case when A can have complex conjugate eigenvalues, and we also provide a method for carrying out the computation and controlling the errors. There are many other ways of constructing invariant manifolds; see e.g. [4–6]. The advantage of the method presented here is that it is simple and can easily be implemented on a computer, see also [12]. The following theorem addresses the problem of computing the unstable manifold tangent to the eigenvector corresponding to a simple real eigenvalue.

Theorem 2. *If A admits a real, simple, strictly positive eigenvalue λ with corresponding eigenvector v and $z : (-1, 1) \rightarrow \mathbb{R}^N$ satisfies $z(0) = 0$ and*

$$(2.2) \quad \lambda s z'(s) = Az(s) + B(sv + z(s))$$

and

$$(2.3) \quad y(t) = e^{\lambda t}v + z(e^{\lambda t})$$

satisfies $y(t) \in D$ for all $t < 0$, then $y(t)$ is a solution of (2.1) for $t < 0$ and $y(t) = e^{\lambda t}v + O(e^{2\lambda t})$ as $t \rightarrow -\infty$.

Remark 1. *The statement of this theorem could be rephrased by saying that $y(t)$ is a parametrization one branch of the unstable manifold at 0 of (2.1). By adapting the proof, one can show that the other branch can be parametrized by $y(t) = -e^{\lambda t}v + z(-e^{\lambda t})$.*

Proof. Consider the change of variable

$$(2.4) \quad s = e^{\lambda t},$$

and write $y(t) = \tilde{y}(s) = z(s) + sv$. If z satisfies (2.2), then

$$\lambda s(v + z'(s)) = s\lambda v + Az(s) + B(sv + z(s)),$$

and

$$(2.5) \quad \lambda s\tilde{y}'(s) = A\tilde{y}(s) + B(\tilde{y}(s)).$$

Since $y'(t) = \lambda e^{\lambda t}\tilde{y}(e^{\lambda t}) = \lambda s\tilde{y}'(s)$, then $y(t) = \tilde{y}(e^{\lambda t})$ satisfies (2.1). Furthermore, $y(t) = e^{\lambda t}v + O(e^{2\lambda t})$ as $t \rightarrow -\infty$. \square

Next, we extend the method to the unstable manifold corresponding to a pair of complex conjugate eigenvalues. Assume that v and \bar{v} are eigenvectors of A , with eigenvalues λ and $\bar{\lambda}$ and $\text{Im}\lambda \neq 0$. If $\text{Re}\lambda > 0$, then equation (2.1) admits an unstable manifold at 0 tangent to the span of $(\text{Re}v, \text{Im}v)$. In order to compute an explicit expression for such a manifold we use the following theorem:

Theorem 3. *Let $B_1(0)$ be the unit disk in \mathbb{C} centered at 0, assume that*

$$Z : [B_1(0)]^2 \rightarrow \mathbb{C}^N$$

satisfies $Z(s_1, 0) = Z(0, s_2) = 0$ and

$$(2.6) \quad \lambda s_1 Z_1(s_1, s_2) + \bar{\lambda} s_2 Z_2(s_1, s_2) = AZ(s_1, s_2) + B(s_1 v + s_2 \bar{v} + Z(s_1, s_2)),$$

where $Z_k = \frac{\partial Z}{\partial s_k}$. Then, for all $(r_1, r_2) \in [B_1(0)]^2$ and all $t \leq 0$ the function

$$(2.7) \quad y(t) = r_1 e^{\lambda t} v + r_2 e^{\bar{\lambda} t} \bar{v} + Z\left(r_1 e^{\lambda t}, r_2 e^{\bar{\lambda} t}\right)$$

is a solution of equation (2.1). If additionally $r_2 = \bar{r}_1$, then $y(t) \in \mathbb{R}^N$ for all $t \leq 0$.

Remark 2. *The statement of this theorem could be rephrased by saying that for every choice of $(r_1, r_2) \in [B_1(0)]^2$ such that $r_2 = \bar{r}_1$, the function $y(t)$ defined in (2.7) is a parametrization of a curve lying on the stable manifold at 0 of (2.1).*

Proof. Differentiating (2.7) with respect to t we have

$$y'(t) = r_1 \lambda e^{\lambda t} v + r_2 \bar{\lambda} e^{\bar{\lambda} t} \bar{v} + Z_1\left(r_1 e^{\lambda t}, r_2 e^{\bar{\lambda} t}\right) r_1 \lambda e^{\lambda t} + Z_2\left(r_1 e^{\lambda t}, r_2 e^{\bar{\lambda} t}\right) r_2 \bar{\lambda} e^{\bar{\lambda} t}.$$

We also have

$$Ay(t) = r_1 \lambda e^{\lambda t} v + \bar{\lambda} r_2 e^{\bar{\lambda} t} \bar{v} + AZ\left(r_1 e^{\lambda t}, r_2 e^{\bar{\lambda} t}\right),$$

so $y(t)$ is a solution of (2.1) if and only if

$$(2.8) \quad \begin{aligned} & Z_1\left(r_1 e^{\lambda t}, r_2 e^{\bar{\lambda} t}\right) r_1 \lambda e^{\lambda t} + Z_2\left(r_1 e^{\lambda t}, r_2 e^{\bar{\lambda} t}\right) r_2 \bar{\lambda} e^{\bar{\lambda} t} = \\ & AZ\left(r_1 e^{\lambda t}, r_2 e^{\bar{\lambda} t}\right) + B\left(r_1 e^{\lambda t} v + r_2 e^{\bar{\lambda} t} \bar{v} + Z\left(r_1 e^{\lambda t}, r_2 e^{\bar{\lambda} t}\right)\right), \end{aligned}$$

which follows from equation (2.6) by choosing $s_1 = r_1 e^{\lambda t}$ and $s_2 = r_2 e^{\bar{\lambda} t}$. Now set $W(s_1, s_2) = Z(s_2, s_1)$. A direct computation shows that W satisfies

$$(2.9) \quad \lambda s_1 W_2(s_2, s_1) + \bar{\lambda} s_2 W_1(s_2, s_1) = AW(s_2, s_1) + B(s_1 v + s_2 \bar{v} + W(s_2, s_1));$$

if we take the complex conjugate of (2.9) and set $t_1 = \bar{s}_2$ and $t_2 = \bar{s}_1$ we get

$$(2.10) \quad \lambda t_1 \bar{W}_1(\bar{t}_1, \bar{t}_2) + \bar{\lambda} t_2 \bar{W}_2(\bar{t}_1, \bar{t}_2) = A\bar{W}(\bar{t}_1, \bar{t}_2) + \bar{B}(\bar{t}_2 v + \bar{t}_1 \bar{v} + W(\bar{t}_1, \bar{t}_2)).$$

Recalling that B is an analytic function that takes real values for real arguments, we have

$$\bar{B}(\bar{t}_2 v + \bar{t}_1 \bar{v} + W(\bar{t}_1, \bar{t}_2)) = B(t_2 \bar{v} + t_1 v + \bar{W}(\bar{t}_1, \bar{t}_2)),$$

therefore $\bar{W}(\bar{t}_1, \bar{t}_2)$ satisfies equation (2.6). Then $\bar{W}(\bar{t}_1, \bar{t}_2) = Z(t_1, t_2) = \bar{Z}(\bar{t}_2, \bar{t}_1)$, so $Z(s, \bar{s}) = \bar{Z}(s, \bar{s})$ and $y(t)$ takes real values when $r_2 = \bar{r}_1$. \square

It is straightforward to extend Theorem 3 to the case of a manifold of higher dimension, corresponding to real or complex conjugate eigenvalues.

3. ANALYTIC FRAMEWORK

We represent the functions z and Z that are needed for Theorems 2 and 3 as power series. Using the equations (2.2) and (2.6), it is straightforward to determine the coefficients of z and Z recursively. Combining the result with an estimate on the radius of convergence yields the desired parametrization of the invariant manifolds. However, an exact computation of all these coefficients is impossible, except in some very special cases. Besides, the equations involve parameters (eigenvalues and eigenvectors) that may not be computable exactly, depending on the matrix A . The goal therefore is to determine approximate values and rigorous error bounds, first for the eigenvalues and eigenvectors, and then for the Taylor coefficients of z and Z . As can easily be guessed, this goes far beyond what could be done by hand. Fortunately, the most tedious part is trivial enough that it can be done with a computer. But the computer has only a limited number of states and works at a finite speed, so we need a finite (and not too large) dimensional approximation of the problem, with a precise control on the error involved. In Section 4 we describe how to handle this task.

We start by introducing a suitable analytic framework. We discuss here the case of the complex invariant manifold, the other case being simpler.

Let \mathcal{X}_ρ be the space of functions of two complex variables with domain $[B_\rho(0)]^2$, which can be written as a power series

$$(3.1) \quad u(s_1, s_2) = \sum_{j,k=0}^{\infty} u_{jk} s_1^j s_2^k$$

with $u_{jk} \in \mathbb{C}$ and such that

$$\|u\|_\rho := \sum_{j,k=0}^{\infty} |u_{jk}| \rho^{j+k} < +\infty.$$

The following lemma is straightforward:

Lemma 4. *For all $\rho > 0$ the space \mathcal{X}_ρ is a Banach algebra; in particular, for all $u, v \in \mathcal{X}_\rho$ we have $uv \in \mathcal{X}_\rho$ and $\|uv\|_\rho \leq \|u\|_\rho \|v\|_\rho$.*

In order to compute a function in \mathcal{X}_ρ which satisfies the assumptions of Theorem 3, we define \mathcal{Z}_ρ as the subalgebra of the functions in \mathcal{X}_ρ with the coefficients of order 0 and 1 (that is the constant and first order terms) equal to 0, then we define \mathcal{Z}_ρ^N as the Banach space of N -tuples of functions in \mathcal{Z}_ρ with norm

$$\|Z\|_\rho = \sum_{k=1}^N \|Z_k\|_\rho$$

and we write equation (2.6) as

$$(3.2) \quad Z(s_1, s_2) = D_\lambda^{-1}(AZ(s_1, s_2) + B(s_1 v + s_2 \bar{v} + Z(s_1, s_2))),$$

where $Z \in \mathcal{Z}_\rho^3$ and D_λ^{-1} is defined by

$$D_\lambda^{-1}(s_1^j s_2^k) = \frac{s_1^j s_2^k}{j\lambda + k\bar{\lambda}},$$

(we abuse the notation by calling D_λ^{-1} both the operator acting on $s_1^j s_2^k$ and its natural extension to a vector of functions). The equation (3.2) that we need to solve can be written as $Z = \mathcal{C}(Z)$, where

$$\mathcal{C}(Z) = D_\lambda^{-1}(AZ + B(s_1 v + s_2 \bar{v} + Z)).$$

We will restrict our analysis to a small ball $B_r(Z_0)$ in \mathcal{Z}_ρ^3 , centered at an approximate solution Z_0 . The map B considered is essentially a polynomial, except for a factor $[1 - L(Z - Z_0)]^{-1}$, where L is a continuous linear functional that is bounded away from 1 in the ball $B_r(0)$. Thus, by Lemma 4, the map $\mathcal{C} : B_r \rightarrow \mathcal{Z}_\rho^3$ is analytic. And its fixed point is the solution of (3.2) that we are looking for.

What is crucial for our computer-assisted proof is the following:

Lemma 5. *\mathcal{C} is a limit of finite rank operators.*

This follows immediately from the definition of \mathcal{X}_2 and of D_λ^{-1} , together with the continuity of the map $Z(s_1, s_2) \mapsto (AZ(s_1, s_2) + B(s_1 v + s_2 \bar{v} + Z(s_1, s_2)))$.

A common method for solving the fixed point problem for a smooth map like \mathcal{C} is the Newton-like iteration $z \mapsto \mathcal{C}(z) - [D(\mathcal{C}(z) - I)]^{-1}(\mathcal{C}(z) - z)$, where D denotes the differential and I the identity operator. Thanks to the above-mentioned property of \mathcal{C} , we can replace the the derivative $D(\mathcal{C}(z) - I)$ by a finite rank approximation. To this end, we consider an m -dimensional subspace \mathbb{C}_m of \mathcal{Z}_ρ^3 , obtained via a projection $P : \mathcal{Z}_\rho^3 \rightarrow \mathbb{C}_m$ that truncates high order Taylor coefficients. Identifying \mathbb{C}_m with \mathbb{C}^m , we choose an invertible $m \times m$ matrix M that approximates $[D(PCP) - I]^{-1}$, where D denotes the Jacobian and I the $m \times m$ identity matrix. Fix $\rho > 0$ and let $\mathcal{N} : \mathcal{Z}_\rho^3 \rightarrow \mathcal{Z}_\rho^3$ be defined by

$$\mathcal{N}(Z) = \mathcal{C}(Z) - MP(\mathcal{C}(Z) - Z);$$

clearly, if the operator $I - MP$ is invertible, or equivalently, if the matrix $I_n - M$ is invertible, then fixed points of \mathcal{N} correspond to fixed points of \mathcal{C} . A direct consequence of the contraction theorem is the following

Lemma 6. *If there exist positive constants ε, r, K and $Z_0 \in \mathcal{Z}_\rho^3$ such that*

- $\|\mathcal{N}(Z_0) - Z_0\|_\rho < \varepsilon$,
- $\|DN(Z)\|_\rho \leq K$ for all $Z \in B_r(Z_0)$, where here $\|\cdot\|_\rho$ denotes the operator norm inherited from \mathcal{Z}_ρ^3 ,
- $\varepsilon + rK < 1$,

then there exists a unique fixed point of \mathcal{N} in $B_r(Z_0)$.

4. THE COMPUTER ASSISTED PROOF

4.1. The differential equation. If we set $y = (v, z, w)$,

$$(4.1) \quad A_c = \begin{pmatrix} 0 & 1 & 0 \\ \alpha & -c\varepsilon & 1 \\ -1/c & 0 & 1/(c\tau) \end{pmatrix} \quad \text{and} \quad B_c(v, z, w) = \begin{pmatrix} 0 \\ b_2(v, z, w) \\ b_3(v, z, w) \end{pmatrix}$$

with

(4.2)

$$b_2(v, z, w) = c\varepsilon\beta v z(3 - 2\beta v) - \frac{\beta z^2}{1 - \beta v} + (v^5\beta^2 - v^4\alpha\beta^2 - v^4\beta^2 - 2v^4\beta \\ + v^3\alpha\beta^2 + 2v^3\alpha\beta + 2v^3\beta + v^3 - 2v^2\alpha\beta - v^2\alpha - v^2) + (\beta^2v^2 - 2\beta v)w, \\ b_3(v, z, w) = \frac{\beta w z}{1 - \beta v}$$

then the system (1.10) takes the form

$$(4.3) \quad y' = A_c y + B_c(y),$$

so we can apply the technique developed in the previous sections. The first step consists in computing the eigenvalues and eigenvectors of A_c ; a direct computation yields:

Lemma 7. *For all $c \in [c_0 - \delta, c_0 + \delta]$ the matrix A_c admits a real eigenvalue $\lambda_1(c) > 0$ and a pair of complex conjugate eigenvalues $\lambda_{2,3}(c) = \lambda_R(c) \pm i\lambda_I(c)$ with $\lambda_R(c) < 0$.*

We compute explicitly such eigenvalues and the corresponding eigenvectors v_j . The following lemmas, whose proof is computer assisted and is described in Section 4, provide a local parametrization of both the stable and the unstable manifold at 0.

Lemma 8. *There exist coefficients $z_k(c)$ depending on c and a positive real number E such that*

$$z_c(s) = \sum_{k=2}^{100} z_k(c)s^k + E_z(s),$$

is a solution of eq. (2.2) for all $c \in [c_0 - \delta, c_0 + \delta]$, where the matrix A is given in (4.1), B is given in (4.2), λ, v are the real eigenvalue/vector of A_c and E_z is a truncation error satisfying $\|E_z\|_{1/4} < E$.

By Theorem 2 it follows that the function $z_c(s) + sv$ is a parametrization of the section close to the origin of the unstable manifold at 0 of (4.3). It turns out that such parametrization only covers a small section of the unstable manifold. To extend it we set $y_0(c) = z_c(1/4) + (1/4)v$, so that $y_0(c)$ is a nontrivial point on the unstable manifold, and then we solve the initial value problem

$$(4.4) \quad \begin{cases} y'_c(t) &= A_c y_c(t) + B_c(y_c(t)) \\ y_c(0) &= y_0(c) \end{cases}$$

for $t \in [0, 203/4]$, since numerical estimates show that $y_c(203/4)$ is very close to the origin. To solve (4.4) we define the operator D_y^{-1} by

$$(D_y^{-1}z)(t) = \int_y^t z(s) ds,$$

we set $C(z) = D_{y_0(c)}^{-1}(A_c z + B_c(z))$ and we look for a fixed point of C . In this case, we do not need a Newton map, since the operator C turns out to be a contraction.

Lemma 9. *There exist coefficients $z_k(c)$ depending on c and a positive real number E such that*

$$z_c(s) = \sum_{k=0}^{100} z_k(c) s^k + E_z(s)$$

with $\|E_z\|_1 < E$ is a solution of (4.4).

We set $y_1(c) = z_c(1)$ and we apply again Lemma 9 iteratively, until we obtain a rigorous bound for $y_{45}(c)$. Then, we do the same again, but with the smaller time step $t = 1/16$, until we have a rigorous bound for $\tilde{y}(c) = y_{50+3/4}(c)$. It is necessary to reduce the time step during the final part of the computation in order to achieve a sufficient precision.

Finally, we build a local parametrization of the stable manifold:

Lemma 10. *There exist coefficients $z_{jk}(c)$ depending on c as described above, and a positive real number E such that*

$$Z(s_1, s_2, c) = \sum_{\substack{j+k \leq 30 \\ j, k \geq 0}} z_{jk}(c) s_1^j s_2^k + E_Z(s_1, s_2),$$

$\|E_Z\|_{3/128} < E$, is a solution of eq. (2.6).

By Theorem 3 (see also Remark 2), the function $Z(x+iy, x-iy, c)$, with $x^2+y^2 \leq (3/128)^2$, is a parametrization of the stable manifold at 0 of (4.4), close to the origin. Once we have accurate bounds on the local stable and unstable manifolds, we verify the following estimates with the aid of the computer.

Lemma 11. *Let $\tilde{y}(c)$ be as above, $a_1 = 0.0005$, $a_2 = 0.01$ and $a_3 = 1/256$. Let $Z(s_1, s_2, c)$ be as in Lemma 10. There exists a coordinate system in \mathbb{R}^3 such that, if P_j is the projection on the j -th coordinate, then*

- (1) $P_1(\tilde{y}(c_0 - \delta)) < -a_1$ and $P_1(\tilde{y}(c_0 + \delta)) > a_1$.
- (2) $|P_2(\tilde{y}(c))|^2 + |P_3(\tilde{y}(c))|^2 < a_2$ for all c .
- (3) $|P_1(Z(s, \bar{s}, c))| < a_1$ for all $|s| \leq a_3$ and all c .
- (4) Let $C_c = \{x \in \mathbb{R}^3 : x = Z(s, \bar{s}, c), |s| = a_3\}$ and $B = \{x \in \mathbb{R}^3 : |P_2(x)|^2 + |P_3(x)|^2 \leq a_2\}$. For all c we have $C_c \cap B = \emptyset$ and the set C_c is not contractible to a point in $\mathbb{R}^3 \setminus B$.

The above lemma imply the following

Lemma 12. *There exists $c \in (c_0 - \delta, c_0 + \delta)$ and $s \in \mathbb{C}$, $|s| < 3/128$ such that $u(c) = Z(s, \bar{s}, c)$.*

Proof. By (4) the cylinder B is split in (at least) two disjointed parts by the set $S = \{x \in \mathbb{R}^3 : x = Z(s, \bar{s}, c), |s| \leq a_3, |c - c_0| \leq \delta\}$. By (3) the set $S \cap B$ lies between the planes $\Pi^\pm = \{x \in \mathbb{R}^3 : P_1(x) = \pm a_1\}$. By (2), $\tilde{y}(c) \in B$ for all c , and by (1) $\tilde{y}(c_0 - \delta)$ lies below the plane Π^- and $\tilde{y}(c_0 + \delta)$ lies above the plane Π^+ . The assertion follows. \square

By Lemma 12 the manifolds intersect and Theorem 1 follows.

4.2. More on the computer-assisted proof. Here we describe some of the details of our computer-assisted proof of Lemmas 8, 9, 10 and 11. Given the Taylor polynomials and the matrices M (obtained from purely numerical computations), the proofs are clearly a sequence of trivial estimates, assuming that there are no fundamental obstructions. The sequence is finite, as one would expect from Lemma 5. But the steps are much too numerous to be carried out by hand, so we enlist the help of a computer. For the types of operations needed here, the techniques are quite standard by now. Thus, we will restrict our description mainly to the problem-specific parts.

As with any lengthy task, proper organization is crucial. We start by associating to a space X a collection $\text{Std}(X)$ of subsets of X , that are representable on the computer. These sets will be referred to as “standard sets” for X . A “bound” on an element $s \in X$ is then a set $S \in \text{Std}(X)$ containing s . Each collection $\text{Std}(X)$ corresponds to a data type in our programs. Unless stated otherwise, $\text{Std}(X \times Y)$ is taken to be the collection of all sets $S \times T$ with $S \in \text{Std}(X)$ and $T \in \text{Std}(Y)$.

Our standard sets for \mathbb{R} are associated with a data type **Ball**, which consists of pairs $\mathbf{S}=(\mathbf{S.C}, \mathbf{S.R})$, where **S.C** is a representable number (**Rep**) and **S.R** a nonnegative representable number (**Radius**). The standard set defined by a **Ball** \mathbf{S} is the interval $\mathcal{B}(\mathbf{S}) = \{s \in \mathbb{R} : |s - \mathbf{S.C}| \leq \mathbf{S.R}\}$.

For non-representable system parameters, such as the constants appearing in the statement of Theorem 1 (with the exception of δ), we use sets of type **Ball** that contain the given values.

A function Z in \mathcal{X}_ρ admits a Taylor expansion

$$(4.5) \quad Z(s_1, s_2) = \sum_{j,k \geq 0}^{j+k \leq M} z_{jk} s_1^j s_2^k + E_Z,$$

with a remainder $E_Z \in \mathcal{X}_\rho$ whose derivatives $\partial_{s_1}^j \partial_{s_2}^k E_Z$ of order $j+k \leq M$ vanish at the origin. Our standard sets for \mathcal{X}_ρ are represented accordingly, by a type **Taylor2** consisting of a pair $\mathbf{F}=(\mathbf{F.C}, \mathbf{F.E})$, where **F.C** is a two-dimensional array with elements of type **Ball**, and **F.E** is a **Ball**. The array elements $\mathbf{F.C}(\mathbf{I}, \mathbf{J})$ represent bounds on the coefficients z_{jk} in equation (4.5), and **F.E** represents a bound on the norm $\|E_Z\|_\rho$. Analytic functions of a single variable are represented analogously, using a data type **Taylor**.

For the representable numbers, we choose a numeric data type (renamed to **Rep**) for which elementary operations are available with controlled rounding. This makes it possible to implement a bound **Sum** on the function $(s, t) \mapsto s + t$ on $\mathbb{R} \times \mathbb{R}$, as well as bounds on other elementary functions on \mathbb{R} or \mathbb{R}^N , including operations like the matrix product.

Here, a bound on a map $f : X \rightarrow Y$ is a map $F : D_F \rightarrow \text{Std}(Y)$, with domain $D_F \subset \text{Std}(X)$, such that $f(s) \in F(S)$ whenever $s \in S \in D_F$. Such bounds are implemented as procedures or functions in our programs. This can be done hierarchically. Using e.g. the **Sum** for the type **Ball**, it is straightforward to implement a bound **Sum** on the map $(g, h) \mapsto g + h$ from $\mathcal{Z}_\rho \times \mathcal{Z}_\rho$ to \mathcal{Z}_ρ . Similarly for maps like $u \mapsto \|u\|$ or D^{-1} . Implementing a bound on the product $(g, h) \mapsto gh$ is a bit more tedious, but straightforward.

In order to estimate $\|DN(h)\|$ we use the following fact. If L is a continuous linear operator on a Banach space of vectors $u = \sum_k c_k v_k$ with norm $\|u\| = \sum_k \rho_k |c_k|$,

then

$$\|L\| = \sup_k \|Le_k\|, \quad e_k = \rho_k^{-1} v_k.$$

This explicit expression for $\|L\|$ is our main reason for working with a weighted ℓ^1 norm. For the operator $L = DN(h)$, we estimate $\|Le_k\|$ explicitly for $k \leq m$, and then show that $\|Lu\| \leq \delta < 1$ for all functions $u = \sum_{k>m} c_k v_k$ of norm $\|u\| \leq 1$. For the chosen value of m , the set of all such functions u is among the sets in $\text{Std}(\mathcal{Z}_\rho^3)$, so estimating the norm of $DN(h)$ reduces to a finite computation.

An important aspect of our proof is that all computations and estimates have to be carried out for a continuous range of values of the parameter c . This issue is usually addressed with interval arithmetic: In our setting, we could represent c as a `Ball` with center c_0 and radius δ . However, this fails drastically in the given problem, even if the interval $[c_0 - \delta, c_0 + \delta]$ is partitioned into a large number of subintervals: If one attempts to follow the unstable manifold using a parameter of finite width, the errors accumulate very rapidly, and the computation gets quickly out of hand. Therefore, instead of an interval enclosure for c , we use a type `TBall`, which is a `Taylor` of order 2 (a quadratic polynomial plus a remainder). So every `Scalar` is effectively a function of c . To be more precise, we write

$$c = c_0 + \delta\xi,$$

and the actual variable used is not c , but ξ , where $|\xi| \leq 1$. By using `TBalls` as coefficients for the previously discussed algorithm, we obtain an explicit expression for a parametrization of the invariant manifolds, depending on both a geometric parameter and ξ .

For a precise and complete description of all definitions and estimates, we refer to the source code and input data of our computer programs [1]. The source code is written in Ada2005. For the type `Rep` we use a MPFR floating point type, with 128 or 256 mantissa bits, depending on the program. MPFR is an open source multiple-precision floating-point library that supports controlled rounding. Our programs were run successfully on a standard desktop machine, using a public version of the gcc/gnat compiler.

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REFERENCES

- [1] The computer programs are available at http://www.ma.utexas.edu/mp_arc 12-10
- [2] D. Ambrosi, G. Arioli, F. Nobile, A. Quarteroni, *Electromechanical Coupling in Cardiac Dynamics: The Active Strain Approach*, SIAM J. Appl. Math., 71:605-621 (2011).
- [3] G. Arioli, H. Koch, *Computer-assisted methods for the study of stationary solutions in dissipative systems, applied to the Kuramoto-Sivashinski equation* Arch. Ration. Mech. Anal. 197 (2010), no. 3, 1033-1051.
- [4] X. Cabré, E. Fontich, R. de la Llave, *The parameterization method for invariant manifolds. I. Manifolds associated to non-resonant subspaces*. Indiana Univ. Math. J. 52 (2003), no. 2, 283-328
- [5] X. Cabré, E. Fontich, R. de la Llave, *The parameterization method for invariant manifolds. II. Regularity with respect to parameters*. Indiana Univ. Math. J. 52 (2003), no. 2, 329-360
- [6] X. Cabré, E. Fontich, R. de la Llave, *The parameterization method for invariant manifolds. III. Overview and applications*. J. Differential Equations 218 (2005), no. 2, 444-515

- [7] C. Cherubini, S. Filippi, P. Nardinocchi, and L. Teresi, *An electromechanical model of cardiac tissue: Constitutive issues and electrophysiological effects*, Progr. Biophys. Molec. Biol., 97:562-573 (2008).
- [8] T. Johnson, W. Tucker, *A Note on the Convergence of Parametrised Non-Resonant Invariant Manifolds*, Qual. Theory Dyn. Syst. (2011) 10:107–121
- [9] Keener, J. and Sneyd, J., *Mathematical Physiology*, Springer (1998).
- [10] I-Shih Liu, *Continuum Mechanics*, Springer (2002).
- [11] Whiteley, J.P., Bishop, M.J. and Gavaghan, D.J., *Soft tissue modelling of cardiac fibers for use in coupled mechano–electric simulations*, Bull. Math. Biol., 69:2199–2225 (2007).
- [12] A. Wittig, *Rigorous High-Precision Enclosures of Fixed Points and Their Invariant Manifolds*, PhD dissertation (2011), <http://bt.pa.msu.edu/wittigphd>