Accurate Computation and Continuation of Homoclinic and Heteroclinic Orbits for Singular Perturbation Problems

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Accurate Computation and Continuation of Homoclinic and Heteroclinic Orbits for Singular Perturbation Problems

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0. Introduction.

This project has been motivated by the study of turbulent fluid boundary layers in the wall region (Aubry et al. [1]). Numerical investigations of models for the dynamics of fluctuations in the boundary layer reveal the presence of intermittent solutions ("bursts") that are persistent over a range of parameter values in the model and that correspond to heteroclinic cycles in the model equations. Armbruster et al. [2] concluded, using the dynamical systems analysis, that these intermittent solutions of the model are an essential feature and not accidental.

In earlier papers [7, 8, 10, 11, 16] Doedel and Friedman have developed an accurate, robust, and systematic method for computing branches of homoclinic and heteroclinic orbits. These are orbits of an infinite period connecting two fixed points of an associated system of autonomous ordinary differential equations. Homoclinic orbits have been shown to play a fundamental role in phenomena such as bursting in biology, chaotic vibrations of structures, chaotic oscillations in chemical reactions, etc. Heteroclinic orbits are equally important in the understanding of the global behavior of dynamical systems and also in the study of wave phenomena in nonlinear parabolic partial differential equations.

The original goal of this project was to accurately compute heteroclinic cycles and to investigate numerically how these cycles evolve as the problem parameters vary in a model 4-dimensional system studied in [1] and [2]. This model system is a singular perturbation problem. Since homoclinic and heteroclinic orbits often arise in the context of singular perturbation problems, this project has evolved into the development of general efficient algorithms for such situations. We developed our algorithms using model 2- and 3- dimensional problems studied by Deng [12].

The organization of the paper is as follows. We first formulate the problem and describe some algorithms for computation of branches of homoclinics and heteroclinics. Then we describe application of these algorithms to several problems of interest.
1. Formulation of the Problem and Review of Some Earlier Results.

In earlier papers [7, 8, 10] Doedel and Friedman have considered the problem of finding a branch of solutions of the system of autonomous ordinary differential equations

\begin{align}
\text{a)} \quad u'(t) - f(u(t), \lambda) &= 0, \quad u(\cdot), f(\cdot, \cdot) \in \mathbb{R}^n, \quad \lambda \in \mathbb{R}^{n_\lambda}, \\
\text{b)} \quad \lim_{t \to -\infty} u(t) &= u_0, \quad \lim_{t \to \infty} u(t) = u_1.
\end{align}

(1.1)

The method utilizes the linear approximation of the unstable (for \( t < T_- \), \(-T_- > 0\), large) and stable (for \( t > T_+ \), \( T_+ > 0\), large) manifolds, under the assumption that solutions of (1.1) decay exponentially to their limits at \( \pm \infty \). Since every translation of a solution of Eq. (1.1) is also a solution, to remove this “phase” indeterminacy we need to add a constraint. The equation

\[
\int_{-\infty}^{\infty} (f(u(t), \lambda) - f(q(t), \lambda^0)) \cdot \frac{\partial}{\partial t} f(u(t), \lambda) dt = 0
\]

(1.2)

seems to be, computationally, the most appropriate way to do this. It is obtained by requiring that the current solution \( u(t) \) be as “close” as possible to the previously computed solution \( q(t) \) (see [7] for the discussion). Our principle result, Theorem 2 in [10] can be summarized as follows:

\[
\text{Let } (q, \lambda^0) \text{ be a solution of (1.1), (1.2). Assume that } n_\lambda = 2(n_u^- + n_s^+ - n) \geq 0, \text{ where } n_u^- \text{ and } n_s^+ \text{ are dimensions of the unstable and stable manifolds of } u_0 \text{ and } u_1 \text{ respectively. Under appropriate assumptions on } f \text{ and appropriate transversality conditions, in a neighborhood of } (q, \lambda^0) \text{ there exists an unique solution branch } (u(s), \lambda(s)), (u(0), \lambda(0)) = (q, \lambda^0), \text{ of (1.1), (1.2) and for sufficiently large } -T_- > 0, T_+ \text{ an unique branch } (u(s), \lambda_T(s)) \text{ of approximate solutions. Here } s \text{ is the continuation (such as pseudo-arclength, employed by AUTO) parameter.}
\]

Moreover, we have an error estimate

\[
\|\lambda(s) - \lambda_T(s)\|_{\mathbb{R}^{n_\lambda}} + \|u(s) - u_T(s)\|_{W^{1,\infty}(\mathbb{R})} \leq C \left( e^{2T_- \mu_0} + e^{2T_+ \mu_1} \right),
\]

(1.3)

for some \( \mu_0 > 0 > \mu_1 \).

Similar results were obtained in Beyn [3, 4].

In Friedman and Doedel [11] and Friedman [16] the numerical method and its analysis have been extended to the case of center manifolds and higher order approximation of the unstable and stable manifolds.

\textbf{Continuation algorithm 1.} ( [10]). The algorithm is based on the following equations:

\begin{align}
\text{a)} \quad u'(t) - T f(u(t), \lambda) &= 0, \quad 0 < t < 1, \\
\text{b)} \quad f(u_0, \lambda) &= 0, \\
\text{b)} \quad f(u_1, \lambda) &= 0,
\end{align}

(1.4) (1.5)
\begin{align}
\text{(1.6)}
\begin{align*}
a) & \quad f_u(u_0, \lambda)w_{0i} = \mu_{0i}w_{0i}, \quad w_{0i} \in \mathbb{R}^n, \quad \mu_{0i} \in \mathbb{R}, \quad i = 1, \ldots, n_0, \\
b) & \quad f_u(u_1, \lambda)w_{1i} = \mu_{1i}w_{1i}, \quad w_{1i} \in \mathbb{R}^n, \quad \mu_{1i} \in \mathbb{R}, \quad i = 1, \ldots, n_1,
\end{align*}
\end{align}

\begin{align}
\text{(1.7)}
\begin{align*}
a) & \quad |w_{0i}| = 1, \quad i = 1, \ldots, n_0, \\
b) & \quad |w_{1i}| = 1, \quad i = 1, \ldots, n_1,
\end{align*}
\end{align}

\begin{align}
\text{(1.8)}
\int_0^1 \left( f(u(t), \lambda) - f(q(t), \lambda^0) \right) \cdot f_u(u(t), \lambda) f(u(t), \lambda) \, dt = 0,
\end{align}

\begin{align}
\text{(1.9)}
\begin{align*}
a) & \quad u(0) = u_0 + \epsilon_0 \sum_{i=1}^{n_0} c_{0i}w_{0i}, \quad \sum_{i=1}^{n_0} c_{0i}^2 = 1, \\
b) & \quad u(1) = u_1 + \epsilon_1 \sum_{i=1}^{n_1} c_{1i}w_{1i}, \quad \sum_{i=1}^{n_1} c_{1i}^2 = 1.
\end{align*}
\end{align}

Here for \( x, y \in \mathbb{R}^n \) \( x \cdot y \) denotes the inner product in \( \mathbb{R}^n \), and we denote by \( |x| \) the \( l^2 \) norm in \( \mathbb{R}^n \); we shall keep the same notation for the inner product and the norm for finite dimensional Euclidean spaces of dimension other than \( n \). The above equations constitute a system of ordinary differential equations subject to constraints. In concrete cases the number of constraints (and correspondingly, the number of scalar variables) can often be significantly reduced by simple algebra and variations on the normalization equations. Equation (1.4) is the differential equation. It is obtained by truncating (1.1a) to an interval \([T_-, T_+], T_- < 0 < T_+\), setting \( T = |T_-| + T_+ \) and then scaling the independent variable \( t \) so that it varies from 0 to 1. The actual period \( T \) therefore appears explicitly in (1.4), whereas \( T_- \) and \( T_+ \) do not appear explicitly in (1.4) – (1.9). There are \( n_{\lambda} \) problem parameters, viz., \( \lambda_i, i = 1, \ldots, n_{\lambda} \). Equation (1.5) defines two fixed points of the vector field. In (1.6a) we assume that the Jacobian \( f_u(u_0, \lambda) \) has \( n_0 \) distinct real positive eigenvalues \( \mu_{0i} \) with eigenvectors \( w_{0i} \), and \( n - n_0 \) real nonpositive eigenvalues. Similarly, in (1.6b) we assume that the Jacobian \( f_u(u_1, \lambda) \) has \( n_1 \) distinct real negative eigenvalues \( \mu_{1i} \) with eigenvectors \( w_{1i} \), and \( n - n_1 \) real nonnegative eigenvalues. Under appropriate assumptions on \( f \), by the stable manifold theorem the fixed point \( u_0 \) has a (strongly) unstable manifold of dimension \( n_0 \) to which the linear subspace \( S_0 \equiv \text{Span}\{\{w_{0i}\}_{i=1}^{n_0}\} \) is tangent at \( u_0 \). The fixed point \( u_1 \) has a (strongly) stable manifold of dimension \( n_1 \) to which the linear subspace \( U_1 \equiv \text{Span}\{\{w_{1i}\}_{i=1}^{n_1}\} \) is tangent at \( u_1 \).

We have \( w_{0i}, w_{1i}, u_0, u_1 \in \mathbb{R}^n \). Equation (1.9a) then requires that the starting point \( u(0) \) of the orbit \( u(t) \) lie in the tangent manifold \( S_0 \) at "distance" \( \epsilon_0 \) from the fixed point \( u_0 \). Similarly, equation (1.9b) requires the endpoint \( u(1) \) to lie in \( U_1 \) at "distance" \( \epsilon_1 \) from the fixed point \( u_1 \). Finally (1.8) represents the "phase condition".

The unknowns \( u_0 \) and \( u_1 \) can be eliminated entirely from (1.4) – (1.9) by using (1.9). Then (1.4) – (1.8) represent \( n \) coupled differential equations subject to \( n_c = \)}
2n + (n + 1)(n_0 + n_1) + 3 constraints, of which (1.9) is an integral condition. In addition to the vector function variable \( u(t) \in \mathbb{R}^n \) we have scalar variables

\[
\lambda \in \mathbb{R}^{n_\lambda}, \quad \epsilon_0, \epsilon_1 \in \mathbb{R},
\]

\[
\mu_{0i}, c_{0i} \in \mathbb{R}, \quad w_{0i} \in \mathbb{R}^{n}, \quad i = 1, ..., n_0,
\]

\[
\mu_{1i}, c_{1i} \in \mathbb{R}, \quad w_{1i} \in \mathbb{R}^{n}, \quad i = 1, ..., n_1.
\]

The total number of scalar variables equals \( n_v \equiv n_\lambda + (n + 2)(n_0 + n_1) + 2 \). Formally we need \( n_v = n_c - n \) for a single heteroclinic connection. Usually we are interested in computing an entire branch (one dimensional continuum) of orbits, in which case \( n_v = n_c - n + 1 \). This requirement is equivalent to setting the number of free problem parameters

\[
n_\lambda = n - (n_0 + n_1) + 2.
\]

The period \( T \) is kept fixed in the continuation. For \( T \) large and \( \epsilon_0 \) and \( \epsilon_1 \) small, each solution on the branch represents an approximate heteroclinic connection. If we want to increase the period \( T \), then we can replace one of the problem parameters, say \( \lambda_1 \), by \( T \) (see [10] for an example of such a computation).

We formulate the algorithms in the situation when the unstable (stable) manifold is 1-dimensional, while the stable (unstable) manifold can have dimension greater than 1. See also Monteiro [13]. In this case the direction along the unstable (stable) manifold is locally defined by the eigenvector corresponding to the positive (negative) eigenvalue, while it is more difficult to determine what linear combination of eigenvectors defines locally the direction along the stable (unstable) manifold. To be specific and without loss of generality, we assume that the eigenvector $w_0^u$ defines the direction of the one-dimensional unstable manifold $W^u_{loc}(u_0)$ at the fixed point $u_0$.

Starting orbits can be obtained by using either AUTO itself or some initial value solver. In applications we used KAOS [14] and VODE [15].

Continuation algorithm 2 (floating boundary algorithm). Eqs. (1.4) – (1.9) are modified by dropping the equations which define the direction along the stable manifold. The equations now are:

\begin{align}
(2.1) 
& u'(t) - T f(u(t), \lambda) = 0, \quad 0 < t < 1, \\
(2.2) 
& f(u_0, \lambda) = 0, \\
(2.3) 
& f_u(u_0, \lambda) w_0^u = \mu_0^u w_0^u, \quad w_0^u \in \mathbb{R}^n, \quad \mu_0^u \in \mathbb{R}, \\
(2.4) 
& |w_0^u| = 1, \\
(2.5) 
& \int_0^1 (f(u(t), \lambda) - f(q(t), \lambda^0)) \cdot f_u(u(t), \lambda) f(u(t), \lambda) \, dt = 0, \\
(2.6) 
& u(0) = u_0 + \epsilon_0 w_0^u,
\end{align}

The unknown $u_0$ can be eliminated from (2.1)-(2.5) by using (2.6). Then (2.1)-(2.5) represent $n$ coupled differential equations subject to $n_c = 2n + 2$ constraints. In addition to the vector function variable $u(t) \in \mathbb{R}^n$ we have scalar variables

\begin{align}
(2.7) 
& \lambda \in \mathbb{R}^{n_\lambda}, \quad \epsilon_0 \in \mathbb{R}, \\
& \mu_0^u \in \mathbb{R}, \quad w_0^u \in \mathbb{R}^n.
\end{align}
The total number of scalar variables equals \( n_v \equiv n_\lambda + n + 2 \). As in \([7]\) we are interested in computing an entire branch (one dimensional continuum) of orbits, in which case the number of free problem parameters

\[
(2.8) \quad n_\lambda = 1.
\]

**Continuation algorithm 3 (steering vector algorithm).** The equations for this algorithm are:

\[
(2.9) \quad u'(t) - T f(u(t), \lambda) = 0, \quad 0 < t < 1,
\]

\[
(2.10) \quad f(u_0, \lambda) = 0, \\
\quad f(u_1, \lambda) = 0,
\]

\[
(2.11) \quad f_u(u_0, \lambda)w^{u}_0 = \mu^{u}_0 w^{u}_0, \quad w^{u}_0 \in \mathbb{R}^n, \quad \mu^{u}_0 \in \mathbb{R},
\]

\[
(2.12) \quad |d| = 1, \\
\quad |w^{u}_0| = 1,
\]

\[
(2.13) \quad \int_0^1 (f(u(t), \lambda) - f(q(t), \lambda^0)) \cdot f_u(u(t), \lambda)f(u(t), \lambda) \, dt = 0,
\]

\[
(2.14) \quad a) \quad u(0) = u_0 + \epsilon_0 w^{u}_0, \\
\quad b) \quad u(1) = u_1 + \epsilon_1 d, \quad d \in \mathbb{R}^n.
\]

Again the unknowns \( u_0 \) and \( u_1 \) can be eliminated from (2.9)–(2.13), by using (2.14). Then (2.9)–(2.13), represent \( n \) coupled differential equations subject to \( n_\varepsilon = 3n + 3 \) constraints. In addition to the vector function variable \( u(t) \in \mathbb{R}^n \) we have \( n_v \equiv n_\lambda + 2n + 3 \) scalar variables

\[
(2.15) \quad \lambda \in \mathbb{R}^{n_\lambda}, \quad w^{u}_0, \quad d \in \mathbb{R}^n, \quad \epsilon_0, \epsilon_1, \mu^{u}_0 \in \mathbb{R}.
\]

Again we are interested in computing an entire branch (one dimensional continuum) of orbits, in which case we have

\[
(2.16) \quad n_\lambda = 1, \text{ and hence } n_v = 2n + 4.
\]
We next give two algorithms for obtaining starting orbits, which can be used in conjunction with Continuation algorithms 1-3.

**Starting orbit algorithm 1 (IVP Solver)**

**Step 1** Assume that $u_0, w_0^u$, and $\lambda$ are given with $|w_0^u| = 1$. Initialize the “distance” $\epsilon_0$ by “small” number, such as 0.0001 and compute the initial value

\[(2.17) \quad u(0) = u_0 + \epsilon_0 w_0^u.\]

This provides an initial value for an initial value solver such as KAOS [14]. Next solve the initial value problem: \((2.17), (2.18), \)

\[(2.18) \quad u'(t) - Tf(u(t), \lambda) = 0, \quad 0 < t < 1,\]

for “large” time $T$, such as $20 - 100$.

**Step 2** Switch to AUTO. Initialize $u_0, w_0^u, \mu, T$ and $\lambda$ from step 1. Read the data generated by KAOS and interpolate it. This provides an initial orbit $u(t)$ for AUTO.

**Step 3.** Perform continuation by one of the Continuation algorithms 1-3. Note that in the case of the Continuation algorithm 1, one first needs to compute the projection of $u(1)$ found at Step 1 onto the subspace spanned by $w_{1i}$, $i = 1, ..., n_1$.

**Starting orbit algorithm 2 (floating boundary).**

**Step 1.** Initialize the period $T$ by a “small” number, such as 0.01, and the “distance” $\epsilon_0$ by another “small” number, such as 0.0001. Given $u_0$ and $w_0^u$, initialize the solution by a constant:

\[(2.19) \quad u(t) = u_0 + \epsilon_0 w_0^u, \quad 0 < t < 1.\]

**Step 2** Perform continuation in the direction of increasing $T$, while all other parameters are fixed, using the equations

\[(2.20) \quad u'(t) - Tf(u(t), \lambda) = 0, \quad 0 < t < 1,\]

\[(2.21) \quad u(0) = u_0 + \epsilon_0 w_0^u.\]

**Starting orbit algorithm 3 (steering vector).**

**Step 1.** Initialize the period $T$ by a “small” number, such as 0.01, and the “distance” $\epsilon_0$ by another “small” number, such as 0.0001. Given $u_0$ and $w_0^u$, initialize the solution by a constant:

\[(2.22) \quad u(t) = u_0 + \epsilon_0 w_0^u, \quad 0 < t < 1.\]

and initialize $d, \epsilon_1$ from the equations:

\[(2.23) \quad u_1 + \epsilon_1 d = u_0 + \epsilon_0 w_0^u, \quad |d| = 1.\]
Step 2 Perform continuation in the direction of increasing $T$ using the equations

\begin{align}
(2.24) \quad u'(t) - Tf(u(t), \lambda) &= 0, \quad 0 < t < 1, \\
(2.25) \quad a) \quad u(0) &= u_0 + \varepsilon_0 w_0, \\
& \quad b) \quad u(1) = u_1 + \varepsilon_1 d, \quad d \in \mathbb{R}^n, \\
(2.26) \quad |d| &= 1, \\
& \quad |w_0| = 1.
\end{align}

**Remark.** The integral "phase" condition is removed for the *Floating Boundary* and the *Steering Vector* algorithms because its purpose is to prevent the sharp peaks from moving. In this method the peaks must move to approach the heteroclinic orbit from the constant solution. AUTO allows the user to set the accuracy to which the variables and parameters are computed in the continuation procedure, by varying the tolerances. In the beginning of the continuation one must set high tolerances for the parameters and variables, because the constant solution is per se a poor approximation of a heteroclinic orbit.
3. A Model 2-d Singular Perturbation Problem.

3.1 Formulation of the Problem.

The system of equations given below is a model problem which we have used to develop our algorithms in the case of Singular Perturbation Problems,

\[
\begin{align*}
\dot{x} &= (2 - z)a(x - 2) + (z + 2)[\alpha(x - x_0) + \beta(y - y_0)] \\
\dot{y} &= (2 - z)[d(b - a)(x - 2)/4 + by] + (z + 2)[-\beta(x - x_0) + \alpha(y - y_0)] \\
\epsilon \dot{z} &= (4 - z^2)[z + 2 - m(x + 2)] - \epsilon cz
\end{align*}
\]

From Deng [12], it is known that for the parameter values \( a = 1, b = 1.5, c = 2, m = 1.1845, \alpha = 0.01, \beta = 5, x_0 = -0.1, y_0 = -2, \epsilon = 0.01, d = -3.5 \) the solution is a twisted homoclinic orbit, while with the same values of parameters except \( d = -0.2 \) the orbit is nontwisted.

Singular perturbation problems are characterized by the appearance of a small parameter such as \( \epsilon = 0.01 \), which in this case makes the system of ordinary differential equations a stiff system. Stiff equations are systems where the magnitude of one eigenvalue of the Jacobian is considerably greater than the magnitude of the other eigenvalues.

In this system of equations, it is known that a hyperbolic fixed point exists at \( w_0 = (2, 0, -2) \). The eigenvalues of the Jacobian evaluated at \( (2, 0, -2) \) are \( (\mu_1, \mu_2, \mu_3) \approx (-1847, 5, 3) \) with associated eigenvectors \( (w^*_1, w^*_2, w^*_3) \). The eigenvalue \( \mu_1 = -1847 \) is responsible for the stiffness of the system. The eigenvector \( w^*_1 \) gives the local direction of the stable manifold, while some linear combination of \( (w^*_1, w^*_2) \) defines the direction of the unstable manifold.

Computing the homoclinic orbit for the 3-dimensional problem is formidable for 3 reasons: (1) the system of equations in Eq. (3.1) is stiff. (2) It is known theoretically that the direction of the unstable manifold \( W^u_{loc}(w_0) \) is defined only by the eigenvector \( w^*_1 \). However, for the numerically approximate problem (which we solve) both \( w^*_1 \) and \( w^*_2 \) will define the direction of \( W^u_{loc}(w_0) \) and the linear combination of \( w^*_1 \) and \( w^*_2 \) is unknown. (3) There are several heteroclinic orbits near the homoclinic orbit, and the slightest numerical instability will displace the homoclinic orbit to one of these heteroclinic orbits. In view of these reasons, we decided to compute a 2-dimensional homoclinic orbit, to gain some insight into the intricacies of computing the full 3-dimensional orbit. There was also the possibility that we could then compute the 3-d orbit by a homotopy from the 2-d orbit.

For the 2-d problem the stable and unstable manifolds, \( W^s_{loc}(w_0) \) and \( W^u_{loc}(w_0) \) are each one-dimensional.

We attempt to compute homoclinic orbits for the two dimensional system of equations, obtained from Eq. (3.1) by setting \( \dot{y} = 0 \) and \( y = 3.59 \times 10^{-3} \) (since it is known that for the 3-d system \( (x, y, z) = (1.99, 3.59 \times 10^{-3}, -1.99) \) is a fixed point):

\[
\begin{align*}
\dot{x} &= (2 - z)a(x - 2) + (z + 2)[\alpha(x - x_0) + \beta(y - y_0)] \\
\dot{z} &= ((4 - z^2)[z + 2 - m(x + 2)] - \epsilon cz)/\epsilon
\end{align*}
\]
3.2 Computational Results

We use the following notation:

\[ u_0 = (u_{01}, u_{02}) \quad \text{Fixed Point} \]
\[ w_1^u = (w_{11}^u, w_{12}^u) \quad \text{Eigenvector tangent to the unstable manifold at } u_0 \]
\[ w_1^s = (w_{11}^s, w_{12}^s) \quad \text{Eigenvector tangent to the stable manifold at } u_0 \]
\[ d_1 = (d_{11}, d_{12}) \quad \text{Normalized steering vector components connecting } u(1) \text{ and } u_0 \]
\[ \epsilon_0, \epsilon_1 \quad \text{Distance between } u_0 \text{ and } u(0) \]
\[ u_0, w_1^u, w_1^s, d_1, u(0), u(1) \in \mathbb{R}^2 \]
\[ \epsilon_0, \epsilon_1 \in \mathbb{R} \]
\[ \lambda = (\epsilon, d) \in \mathbb{R}^2 \]

To compute a homoclinic orbit for this system of equations we use the steering vector algorithm and after noting that for a homoclinic orbit The homoclinic orbit is obtained for Eq. (3.1) by a series of steps.

**Step 1 (a):** Obtain an initial homoclinic orbit for

(3.3) \[ u' = Tf(u, \lambda), \quad u = (x, z) \]

subject to the boundary conditions:

(3.4) \[
(a) \quad u(0) = u_0 + \epsilon_0 w_1^u \\
(b) \quad u(1) = u_0 + \epsilon_1 d_1
\]

and normalization condition,

(3.5) \[ |d_1| = 1 \]

for a total of 5 boundary conditions. Note that \( d_1 = (d_{11}, d_{12}) \in \mathbb{R}^2 \). Initialize \( T = 0.01, \epsilon_0 = 10^{-7}, u_0 = (1.99, -1.99), w_1^u = (1.0, -5.2 \times 10^{-4}) \) and the tolerances \( \epsilon_u, \epsilon_\lambda = 10^{-2} \). Begin computation of the orbit along the unstable manifold. Perform continuation with respect to \( T, d_{11}, d_{12}, \epsilon_1 \) using the steering vector algorithm for obtaining initial orbits. We have now reached Fig. (3.1), where \( (d = -0.2, \epsilon = 0.01, \epsilon_0 = 1.0 \times 10^{-6}, T = 1.15 \times 10^{-2}, \mu_1^2 = -1891), (\mu_1^u = 3.99, w_{11}^u = 0.99, w_{12}^u = -5.0 \times 10^{-4}), (\epsilon_1 = 1.0 \times 10^{-6}, d_{11} = -0.99, d_{12} = 5.2 \times 10^{-4}), (u_{01} = 1.99, u_{02} = -1.99). \)
Step 1 (b): Decrease the tolerances so that $\epsilon_u, \epsilon_\lambda = 10^{-8}$. Perform continuation with respect to $T, d_{11}, d_{12}, \epsilon_1$ until $d_1$ has approximately the same direction as the eigenvector $w_1^u$, which defines the direction of the stable manifold $W_{loc}^s(u_0)$ near the fixed point. The computation reaches Fig. (3.2) where $\epsilon_1 = 0.078$. In Fig. (3.2) ($d = -0.2, \epsilon = 0.01, \epsilon_0 = 1.0 \times 10^{-6}, T = 3.89, \mu_1^u = -1891, (\mu_1^u = 3.99, w_{11}^u = 0.99, w_{12}^u = -5.0 \times 10^{-4}), (\epsilon_1 = 0.078, d_{11} = -0.42, d_{12} = 0.90), (u_{01} = 1.99, u_{02} = -1.99)$.

Step 2 (a): Switch from the steering vector algorithm to the eigenvector algorithm on the right boundary (stable manifold). The problem is formulated as follows:

$$u' = Tf(u, \lambda), \quad u = (x, z)$$

with the boundary conditions

$$\begin{align*}
(a) \quad u(0) &= u_0 + \epsilon_0 w_1^u \\
(b) \quad u(1) &= u_0 + \epsilon_1 d_1
\end{align*}$$

eigenvalue problem conditions

$$\begin{align*}
(a) \quad f_u^0 w_1^u &= \mu_1^u w_1^u \\
(b) \quad f_u^0 d_1 &= \mu_1^u d_1
\end{align*}$$

normalization conditions

$$\begin{align*}
(a) \quad |w_1^u| &= 1 \\
(b) \quad |d_1| &= 1
\end{align*}$$

and the fixed point conditions

$$f(u_0, \lambda) = 0$$

We now have a total of 12 boundary conditions. At this point in the computation, the direction of the steering vector is only an approximation to the eigenvector which defines the direction of the stable manifold on the right boundary. Therefore, the tolerances for the state variables and the parameters should be set rather high when switching from the steering vector approximation to the eigenvector approximation. Experimentally we found that we needed $\epsilon_u, \epsilon_\lambda = 1$. Perform a few steps of continuation ($NMX = 5$) with respect to $T, \epsilon, \epsilon_1, d_{11}, d_{12}, w_{11}^u, w_{12}^u, \mu_1^u, \mu_1^u, u_{01}, u_{02}$ for a total of 11 parameters. Note the presence of the singular perturbation parameter $\epsilon$. After this step of continuation, the components $d_{11}, d_{12}$ will be aligned along the direction of the eigenvector, which defines the direction of the stable manifold. We have now reached Fig. (3.3) where $\epsilon_1 = 0.0752$ and $d_1 = (d_{11} = -5.91 \times 10^{-3}, d_{12} = 0.99998)$, is now aligned along the eigenvector $w_1^u$, but
the singular perturbation parameter has changed its value to $\epsilon = 0.011645$. In Fig. (3.3) the parameter values are $(d = -0.2, \epsilon = 0.0116, \epsilon_0 = 1.0 \times 10^{-6}, T = 3.85, \mu_1^\epsilon = -1693)$, $(\mu_1^u = 3.99, w_{11}^u = 0.99, w_{12}^u = -5.89 \times 10^{-4})$, $(\epsilon_1 = 0.07, d_{11} = -5.9 \times 10^{-3}, d_{12} = 0.99)$, $(u_{01} = 1.99, u_{02} = -1.99)$.

**Step 2 (b):** Decrease the tolerances to $\epsilon_u, \epsilon_\lambda = 10^{-8}$ and proceed with continuation as in Step 2(a). The singular perturbation parameter $\epsilon$ increased in value from 0.01 to about 1.11, whence the orbit obtained was homoclinic. At intermediate values of $\epsilon_1$ the orbit is not homoclinic. For example for $\epsilon_1 = 0.371$, the orbit is not homoclinic. The orbit obtained for $\epsilon_1 = 1.117774$ is shown in Fig. (3.4), where it is clear that the orbit is homoclinic. The parameter values in Fig. (3.4) are $(d = -0.2, \epsilon = 1.12, \epsilon_0 = 1.0 \times 10^{-6}, T = 8.75, \mu_1^\epsilon = -11)$, $(\mu_1^u = 2.85, w_{11}^u = 0.99, w_{12}^u = -0.079)$, $(\epsilon_1 = 5.3 \times 10^{-13}, d_{11} = -0.59, d_{12} = 0.80)$, $(u_{01} = 1.20, u_{02} = -1.71)$.

**Step 3:** Attempt to decrease $\epsilon$ back to the value of 0.01. Freeze the period $T$ from Step 2(b) and perform continuation with respect to $\epsilon, \epsilon_0, \epsilon_1, d_{11}, d_{12}, w_{11}^u, w_{12}^u, \mu_1^u, \mu_1^\epsilon, u_{01}, u_{02}$ using the same set of boundary conditions described in Step 2(a). A surprising result was noted: (1) $\epsilon$ returned to a value of 0.011117. (2) $\epsilon_0$ had started at a value $\epsilon_0 = 10^{-6}$ in Step 1, but on this return journey, it reached a value of $\epsilon_0 = -2.0 \times 10^{-12}$ and $\epsilon_1 = 1.117 \times 10^{-9}$. This final orbit is shown in Fig. (3.5). The parameter values in Fig. (3.5) are $(d = -0.2, \epsilon = 0.011, \epsilon_0 = -2.7 \times 10^{-10}, T = 8.75, \mu_1^\epsilon = -1693)$, $(\mu_1^u = 3.99, w_{11}^u = 0.99, w_{12}^u = -5.9 \times 10^{-4})$, $(\epsilon_1 = 1.1 \times 10^{-9}, d_{11} = -5.9 \times 10^{-3}, d_{12} = 0.99)$, $(u_{01} = 1.99, u_{02} = -1.99)$.

**Step 4:** We now attempt to compute a branch of homoclinic orbits with respect to $(d, \epsilon)$. Add the integral phase condition and formulate the problem as follows:

$$u' = Tf(u, \lambda), \quad u = (x, z)$$

with the boundary conditions

$$u(0) = u_0 + \epsilon_0 w_{11}^u$$
$$u(1) = u_0 + \epsilon_1 d_1$$

**eigenvalue problem conditions**

$$f_u^0 w_{11}^u = \mu_1^u w_{11}^u$$
$$f_u^0 d_1 = \mu_1^\epsilon d_1$$

**normalization conditions**

$$|w_{11}^u| = 1$$
$$|d_1| = 1$$
and the fixed point conditions

\begin{align}
(3.15) & 
\begin{align}
& f(u_0, \lambda) = 0 \\
(3.16) & 
\int_{-\infty}^{\infty} \left( f(u(t), \lambda) - f(q(t), \lambda^0) \right) \cdot \frac{d}{dt} f(u(t), \lambda) dt = 0
\end{align}
\end{align}

Now perform continuation with respect to $\epsilon, d, \epsilon_0, \epsilon_1, d_{11}, d_{12}, w_{11}^u, w_{12}^u, \mu_1^u, \mu_1^s, u_01, u_02$. This is now a two parameter continuation problem with respect to the parameters $(\epsilon, d)$. The parameter $d$ starts at $d = -0.2$ and continues on until $d = -8000$ without any significant change in the orbit. The stiffness of the problem is not altered by this variation in the parameter $d$.

3.3 Figures

Fig. 3.1. $(d = -0.2, \epsilon = 0.01, \epsilon_0 = 1.0 \times 10^{-6}, T = 1.15 \times 10^{-2}, \mu_1^s = -1891), (\mu_1^u = 3.99, w_{11}^s = 0.99, w_{12}^u = -5.0 \times 10^{-4}), (\epsilon_1 = 1.0 \times 10^{-6}, d_{11} = -0.99, d_{12} = 5.2 \times 10^{-4}), (u_{01} = 1.99, u_{02} = -1.99)$.

Fig. 3.2. $(d = -0.2, \epsilon = 0.01, \epsilon_0 = 1.0 \times 10^{-6}, T = 3.89, \mu_1^s = -1891), (\mu_1^u = 3.99, w_{11}^s = 0.99, w_{12}^u = -5.0 \times 10^{-4}), (\epsilon_1 = 0.078, d_{11} = -0.42, d_{12} = 0.90), (u_{01} = 1.99, u_{02} = -1.99)$.

Fig. 3.3. $(d = -0.2, \epsilon = 0.0116, \epsilon_0 = 1.0 \times 10^{-6}, T = 3.85, \mu_1^s = -1693), (\mu_1^u = 3.99, w_{11}^s = 0.99, w_{12}^u = -5.89 \times 10^{-4}), (\epsilon_1 = 0.07, d_{11} = -5.9 \times 10^{-3}, d_{12} = 0.99), (u_{01} = 1.99, u_{02} = -1.99)$.

Fig. 3.4. $(d = -0.2, \epsilon = 1.12, \epsilon_0 = 1.0 \times 10^{-6}, T = 8.75, \mu_1^s = -11), (\mu_1^u = 2.85, w_{11}^s = 0.99, w_{12}^u = -0.079), (\epsilon_1 = 5.3 \times 10^{-13}, d_{11} = -0.59, d_{12} = 0.80), (u_{01} = 1.20, u_{02} = -1.71)$.

Fig. 3.5. $(d = -0.2, \epsilon = 0.011, \epsilon_0 = -2.7 \times 10^{-10}, T = 8.75, \mu_1^s = -1693), (\mu_1^u = 3.99, w_{11}^s = 0.99, w_{12}^u = -5.9 \times 10^{-4}), (\epsilon_1 = 1.1 \times 10^{-9}, d_{11} = -5.9 \times 10^{-3}, d_{12} = 0.99), (u_{01} = 1.99, u_{02} = -1.99)$. 

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FIGURE 3.1
FIGURE 3.2
FIGURE 3.2 (Con't.)
FIGURE 3.3
FIGURE 3.3 (Con't.)
FIGURE 3.3 (Con't.)
FIGURE 3.4
FIGURE 3.4 (Con't.)
FIGURE 3.4 (Con't.)
ERROR - REENTER TWO AXIS
DEFAULT AXES ARE:
2 3
LABELS HAVE DIMENSION
3
DIMENSION : 3
ENTER AXES (DEFAULT 2 3), <D> (DISPLAY), OR <EX> (EXIT)
2d
THE LABELS ARE:
1 2 3 4 5 6 7 8 9 10
11 12 13 14 15 16 17 18 19 20
21 22 23 24 25 26 27 28 29 30
31 32 33 34 35 36 37 38 39 40
41 42 43 44 45 46 47 48 49

FIGURE 3.4 (Con't.)
FIGURE 3.4 (Con't.)
FIGURE 3.5
4. A Model 3-d Singular Perturbation Problem

4.1 Formulation of the Problem

The system of equations given below is the model problem for applying continuation algorithms to Singular Perturbation Problems,

\[
\begin{align*}
\dot{x} &= (2 - z)\alpha(x - 2) + (z + 2)[\alpha(x - x_0) + \beta(y - y_0)] \\
\dot{y} &= (2 - z)[d(b - a)(x - 2)/4 + by] + (z + 2)[-\beta(x - x_0) + \alpha(y - y_0)] \\
\epsilon \dot{z} &= (4 - z^2)[z + 2 - m(x + 2)] - \epsilon cz
\end{align*}
\] (4.1)

From Deng [12], it is known that for the parameter values \(a = 1, b = 1.5, c = 2, m = 1.1845, \alpha = 0.01, \beta = 5, x_0 = -0.1, y_0 = -2, \epsilon = 0.01, d = -3.5\) the solution is a twisted homoclinic orbit, while with the same values of parameters except \(d = -0.2\) the orbit is nontwisted.

Singular perturbation problems are characterized by the appearance of a small parameter such as \(\epsilon = 0.01\), which in this case makes the system of ordinary differential equations stiff. Stiff equations are systems where the magnitude of one eigenvalue of the Jacobian is considerably greater than the magnitude of the other eigenvalues.

In this system of equations, it is known [12] that there exists a hyperbolic fixed point near \(u_0 = (2, 0, -2)\) for \((\epsilon, d) = (0.01, -0.2)\). A more accurate solution with the IMSL subroutine DNEQNF yields \(u_0 = (1.99469, 3.59524 \times 10^{-3}, -1.997886)\) for Eq. (4.1). The eigenvalues of the Jacobian evaluated at \(u_0\) are \((\mu_1^s, \mu_1^u, \mu_2^u) \approx (-1891, 3.99, 5.99)\) with associated eigenvectors \(w_1^s = (-5.3 \times 10^{-3}, 5.5 \times 10^{-3}, 0.99)\), \(w_1^u = (0.99, 5.2 \times 10^{-2}, -5.2 \times 10^{-4})\), \(w_2^u = (5.2 \times 10^{-3}, 0.99, -2.7 \times 10^{-6})\). The eigenvalue \(\mu_1^s = -1891\) is responsible for the stiffness of the system. The eigenvector \(w_1^s\) gives the local direction of the stable manifold \(W_{loc}^s(u_0)\), while some linear combination of \((w_1^s, w_1^u)\) defines the direction of the unstable manifold \(W_{loc}^u(u_0)\).

To compute the non-twisted homoclinic orbit, we used the steering vector algorithm. The boundary \(u(0)\) was displaced from the fixed point \(u_0\) by \(\epsilon_0\) along the eigenvector \(w_1^u\) as outlined in [13]; this corresponded to the unstable manifold. The boundary \(u(1)\) was attached to the steering vector \(d_1\). The results of the computation are shown in the attached Figures.

4.2 Computational Results.

Drawing on insight obtained from the two dimensional problem, we attempted to compute homoclinic orbits for the three dimensional system:

\[
u' = T'f(u, \lambda), \ u = (x, y, z)
\] (4.2)

which symbolically represent Eq. (4.1). To compute a homoclinic orbit for this system of equations, we will go through a number of steps, with each step having a different set of boundary conditions.
We use the following notation:

\[ u_0 = (u_{01}, u_{02}, u_{03}) \quad \text{Fixed Point} \]
\[ w_1^u = (w_{11}^u, w_{12}^u, w_{13}^u) \quad \text{First eigenvector tangent to the unstable manifold at } u_0 \]
\[ w_2^u = (w_{21}^u, w_{22}^u, w_{23}^u) \quad \text{Second eigenvector tangent to the unstable manifold at } u_0 \]
\[ w_1^s = (w_{11}^s, w_{12}^s, w_{13}^s) \quad \text{Eigenvector tangent to the stable manifold at } u_0 \]
\[ d_1 = (d_{11}, d_{12}, d_{13}) \quad \text{Normalized steering vector components connecting } u(1) \text{ and } u_0 \]
\[ \epsilon_0 \quad \text{Distance between } u_0 \text{ and } u(0) \]
\[ \epsilon_1 \quad \text{Distance between } u_0 \text{ and } u(1) \]

**Step 1 (a):** Initialize \( T = 0.01, \epsilon_0 = 10^{-7}, (\epsilon, d) = (0.01, -0.2) \) and set the tolerances to \( \epsilon_u, \epsilon_\lambda = 10^{-2} \). We attempt to start computing the homoclinic orbit along the unstable manifold \( W_{loc}^u(u_0) \) from the boundary \( u(0) \). \( W_{loc}^u(u_0) \) is defined by some linear combination of the eigenvectors, \((w_1^u, w_2^u)\). This linear combination is not known *a priori*, so following Deng [12] we start the computation of the orbit along the eigenvector \( w_1^u \). We obtain an initial orbit for Eq. (4.1) formulated as follows:

\[
(4.3) \quad u' = Tf(u, \lambda), \quad u = (x, y, z)
\]

with the 6 boundary conditions,

\[
(4.4) \quad (a) \ u(0) = u_0 + \epsilon_0 \{w_1^u \cos \kappa + w_2^u \sin \kappa\}
\]
\[
(b) \ u(1) = u_0 + \epsilon_1 d_1
\]

and normalization condition,

\[
(4.5) \quad |d_1| = 1
\]

Note that \( d_1 = (d_{11}, d_{12}, d_{13}) \). Perform continuation with respect to \( T, \epsilon_1, d_{11}, d_{12}, d_{13} \) using the steering vector algorithm for obtaining an initial orbit as described in [13]. Typically, we use \( NMX = 5 \) with \( NBC = 7, NINT = 0, NTST = 25, NCOL = 5 \).

**Remark:** At Step 1(a), we assume that the solution to Eq. (4.3) remains constant over the interval \( T = 0.01 \). The tolerances are set to the high value \( \epsilon_u, \epsilon_\lambda = 10^{-2} \) in the event that the assumption is not true and the solution does vary substantially.

Once the solution reaches Fig. (4.1), AUTO will have computed an accurate enough solution, so that the next step of computation can proceed with much lower tolerances. In fact, in the next step, all we do is to lower the tolerances.

**Step 1 (b):** At this point AUTO has been able to find an initial orbit, so we decrease the tolerances to \( \epsilon_u, \epsilon_\lambda = 10^{-8} \). Perform continuation with respect to \( T, \epsilon_1, d_{11}, d_{12}, d_{13}, \)
using the same set of boundary conditions as in Step 1(a) until \( d_1 \) has approximately the same direction as the eigenvector \( w^1_1 \), which defines the direction of the stable manifold near the fixed point. In Fig. (5.2) \( T = 4.3, \epsilon_1 = 0.3, d_1 = (7.5 \times 10^{-3}, -2.9 \times 10^{-3}, 0.95) \) and this is a fairly good approximation to the eigenvector \( w^1_1 = (-5.3 \times 10^{-3}, 5.5 \times 10^{-3}, 0.99) \), which defines the direction of the stable manifold, \( W^2_{loc}(u_0) \). At this point we still use pseudo-arclength continuation with \( NBC = 7, NINT = 0, NTST = 25, NCOL = 5 \). We now attempt to switch from the steering vector to the eigenvector approximation at the boundary \( u(1) \).

**Remark**: It is important to watch the continuation process very carefully in Step 1(b) to see when \( d_1 \), is approximately aligned along the eigenvector \( w^1_1 \). Fig. (4.3a), shows what happens when \( u(1) \) is “too close” to the fixed point for this stage of the continuation (\( \epsilon_1 = 0.1 \)), but \( d_1 = (0.04, -0.99, -2.2 \times 10^{-5}) \) is a hopeless approximation to \( w^1_1 = (-5.3 \times 10^{-3}, 5.5 \times 10^{-3}, 0.99) \). We used the 7 boundary conditions of Step 1(b), and attempted to perform continuation with respect to \( T, \kappa, d_{11}, d_{12}, d_{13} \) in the hope that the steering vector \( d_1 \) would align along the eigenvector \( w^1_1 \) for some value of \( \kappa \). Unfortunately, this was not the case. Once \( y(t) \) undershoots (falls below the fixed point value on the right boundary \( u(1) \)) as shown in Fig. (4.3b), it is impossible to compute the homoclinic orbit, no matter how close one is to the fixed point.

**Step 2 (a)**: Switch from the steering vector algorithm to the eigenvector algorithm on the right boundary (stable manifold). i.e. Solve the following equation:

\[
\dot{u} = Tf(u, \lambda), \; u = (x, y, z)
\]

with the 6 boundary conditions,

\[
(a) \; u(0) = u_0 + \epsilon_0 \{ w^u_1 \cos \kappa + w^u_2 \sin \kappa \}
(b) \; u(1) = u_0 + \epsilon_1 d_1
\]

9 eigenvalue problem conditions,

\[
(a) \; f^0_u w^u_1 = \mu^u_1 w^u_1
(b) \; f^0_u w^u_2 = \mu^u_2 w^u_2
(c) \; f^0_u d_1 = \mu^u_1 d_1
\]

3 normalization conditions,

\[
(a) \; |w^u_1| = 1
(b) \; |w^u_2| = 1
(c) \; |d_1| = 1
\]

and the 3 fixed point conditions,
We now have a total of 21 boundary conditions. Continuation is carried out with respect to the variables: \( T, \epsilon, (\epsilon_1, d_{11}, d_{12}, d_{13}), (\mu_1^u, w_{11}^u, w_{12}^u, w_{13}^u), (\mu_2^u, w_{21}^u, w_{22}^u, w_{23}^u), (u_{01}, u_{02}, u_{03}), \mu_1^s, \kappa \). At this point in the computation, the steering vector has only approximately the same direction as the eigenvector which defines the direction of the stable manifold on the right boundary. Therefore, the tolerances for the state variables and the parameters should be set rather high when switching from the steering vector approximation to the eigenvector approximation. Experimentally we found that we needed \( \epsilon_u, \epsilon_\lambda = 1 \). Note that Eq. (4.8c) forces a change from the steering vector algorithm to the eigenvector algorithm. After this step of continuation \( d_1 \) is aligned along the direction of the eigenvector \( w_1^u \) which defines the direction of the stable manifold \( W^s_{loc}(u_0) \). We have now reached Fig. (4.4), where \( \epsilon_1 = 0.345 \) and \( d_{11} = -4.87 \times 10^{-3}, d_{12} = 5.06 \times 10^{-3}, d_{13} = 1.0 \) are now aligned along the eigenvector \( w_1^u \), but the singular perturbation parameter has changed its value to \( \epsilon = 0.0092 \). The other parameter values are \( d = -0.2, \epsilon = 9.2 \times 10^{-3}, T = 4.3, \epsilon_0 = 10^{-7}, \epsilon_1 = 0.3, \kappa = 5.7 \times 10^{-4}, (\mu_1^s = -2039, d_{11} = -4.9 \times 10^{-3}, d_{12} = 5.1 \times 10^{-3}, d_{13} = 1.0), (\mu_1^u = 4, w_{11}^u = 0.99, w_{12}^u = 0.05, w_{13}^u = -4.9 \times 10^{-4}), (\mu_2^u = 5.99, w_{21}^u = 4.8 \times 10^{-3}, w_{22}^u = 0.99, w_{23}^u = -2.3 \times 10^{-6}), (u_{01} = 1.99, u_{02} = 3.3 \times 10^{-3}, u_{03} = -1.99). 

Remark: It is also possible to switch from the steering vector approximation to the eigenvector approximation via a homotopy.

**Step 3 (a):** Decrease the tolerances to \( \epsilon_u, \epsilon_\lambda = 10^{-1} \), set \( NTST = 100, NCOL = 5, DS = -1.0 \times 10^{-4} \) and use Natural Parameter Continuation to solve:

\[
(4.11) \quad u' = Tf(u, \lambda), \quad u = (x, y, z)
\]

with the integral phase condition,

\[
(4.12) \quad \int_{-\infty}^{\infty} (f(u(t), \lambda) - f(q(t), \lambda^0)) \cdot \frac{d}{dt} f(u(t), \lambda) dt = 0
\]

the 6 boundary conditions,

\[
(4.13) \begin{align*}
(a) \quad u(0) &= u_0 + \epsilon_0 \{ w_1^u \cos \kappa + w_2^u \sin \kappa \} \\
(b) \quad u(1) &= u_0 + \epsilon_1 d_1
\end{align*}
\]

9 eigenvalue problem conditions,

\[
(4.14) \begin{align*}
(a) \quad f_u^0 w_1^u &= \mu_1^u w_1^u \\
(b) \quad f_u^0 w_2^u &= \mu_2^u w_2^u \\
(c) \quad f_u^0 d_1 &= \mu_1^s d_1
\end{align*}
\]
3 normalization conditions,

\begin{align}
(a) \ |w_u^u| &= 1 \\
(b) \ |w_u^2| &= 1 \\
(c) \ |d_1| &= 1
\end{align}

and the 3 fixed point conditions,

\begin{equation}
\mathbf{f}(u_0, \lambda)
\end{equation}

We now have a total of 21 boundary conditions plus an Integral Phase Condition. Continuation is carried out with respect to the variables: \( \epsilon_1, T, \epsilon, (d_{11}, d_{12}, d_{13}), (\mu_1^u, w_{11}^u, w_{12}^u, w_{13}^u), (\mu_2^u, w_{21}^u, w_{22}^u, w_{23}^u), (u_{01}, u_{02}, u_{03}), \mu_1^s, k, \epsilon_0 \). Note that continuation is carried out with \( \epsilon_1 \) as the primary parameter, which in conjunction with the negative value of \( DS \) and Natural Parameter Continuation, ensures that the length of the steering vector continuously decreases, pulling the orbit towards the fixed point. Note also that \( \epsilon_0 \) and \( \kappa \) are allowed to vary so that the correct linear combination of eigenvectors is found on the two dimensional unstable manifold, \( W_{loc}^{u}(u_0) \) to compute an accurate homoclinic orbit.

In Fig. (4.5), the singular perturbation parameter \( \epsilon = 9.33 \times 10^{-3}, \epsilon_1 = 0.344 \). The parameter values are:

\begin{align*}
d &= -0.2, \epsilon = 9.3 \times 10^{-3}, T = 4.3, \epsilon_0 = 1.9 \times 10^{-7}, \epsilon_1 = 0.34, k = -5 \times 10^{-6}, (\mu_1^s = -2025, d_{11} = -4.9 \times 10^{-3}, d_{12} = 5.1 \times 10^{-3}, d_{13} = 0.99), (\mu_1^u = 4, w_{11}^u = 0.99, w_{12}^u = 0.05, w_{13}^u = -4.9 \times 10^{-4}), (\mu_2^u = 5.99, w_{21}^u = 4.9 \times 10^{-3}, w_{22}^u = 0.99, w_{23}^u = -2.4 \times 10^{-6}), (u_{01} = 1.99, u_{02} = 3.35 \times 10^{-3}, u_{03} = -1.99).
\end{align*}

The next step in the computation is to decrease \( \epsilon_1 \) still more, while simultaneously attempting to increase the accuracy of the computation, which involves decreasing the tolerances \( \epsilon_u, \epsilon_\lambda \).

**Remark:** It was extremely crucial in this step to set \( NTST = 100 \) to carry out the continuation procedure. From the phase space plot of Fig. (4.5), it is clear that there are several sharp fronts, and this high value of \( NTST = 55 \) is the only way to accurately compute the solution with these sharp fronts. For example, a value of \( NTST = 55 \) allowed tolerances of only \( \epsilon_u, \epsilon_\lambda = 1 \) and this was not sufficiently accurate for continuation.

**Step 3(b):** The only change from Step (3a) is that we decrease the tolerances and set \( \epsilon_u, \epsilon_\lambda = 10^{-8} \). The continuation proceeds as before with Natural Parameter Continuation with respect to the same parameters as in Step (3a). We stop the computation at the point shown in Fig. (4.6), where \( \epsilon_0 = 3.7 \times 10^{-9}, \epsilon_1 = 1.0 \times 10^{-7}, \epsilon = 9.3 \times 10^{-3}, T = 5.3 \). The parameter values are:

\begin{align*}
d &= -0.2, \epsilon = 9.3 \times 10^{-3}, T = 5.3, \epsilon_0 = 3.7 \times 10^{-9}, \epsilon_1 = 1.1 \times 10^{-7}, k = -2.7 \times 10^{-7}, (\mu_1^s = -2026, d_{11} = -4.9 \times 10^{-3}, d_{12} = 5.1 \times 10^{-3}, d_{13} = 0.99), (\mu_1^u = 4, w_{11}^u = 0.99, w_{12}^u = 0.05, w_{13}^u = -4.9 \times 10^{-4}), (\mu_2^u = 5.99, w_{21}^u = 4.9 \times 10^{-3}, w_{22}^u = 0.99, w_{23}^u = -2.4 \times 10^{-6}), (u_{01} = 1.99, u_{02} = 3.5 \times 10^{-3}, u_{03} = -1.99).
\end{align*}

**Remark:** The extremely small values of \( \epsilon_0 \) and \( \epsilon_1 \) indicate that the homoclinic orbit has been computed very accurately. In practice, an accuracy of \( \epsilon_0, \epsilon_1 = 1.0 \times 10^{-5} \) should suffice.

**Step 4:** We now attempt to compute a branch of homoclinic orbits with respect to the parameters \((d, \epsilon)\) of Eq. (4.1). Deng [12] notes that the homoclinic orbit is
twisted for \( d = -3.5 \) and non-twisted for \( d = -0.2 \). Consequently, we again use Natural Parameter Continuation to decrease \( d \) from \(-0.2\) to \(-3.5\). We use the same set of boundary conditions as in Step (3a) but perform continuation with respect to \( d, \epsilon, \epsilon_0, (\epsilon_1, d_{11}, d_{12}, d_{13}), (\mu_1^u, w_{11}^u, w_{12}^u, w_{13}^u), (\mu_2^u, w_{21}^u, w_{22}^u, w_{23}^u), (u_{01}, u_{02}, u_{03}), \mu_1^s, \kappa \). This is now a two parameter continuation problem with respect to the parameters \((\epsilon, d)\). The parameter \( d \) starts at \( d = -0.2 \) and continues on until \( d = -3.5 \) with a significant change in the orbit as shown in Fig. (4.7). The parameter values are: \( d = -3.5, \epsilon = 9.3 \times 10^{-3}, \epsilon_0 = 4.7 \times 10^{-9}, \epsilon_1 = 1.1 \times 10^{-7}, \kappa = -1.4 \times 10^{-5}, (\mu_1^u = -2024, d_{11} = -5.3 \times 10^{-3}, d_{12} = 5.5 \times 10^{-3}, d_{13} = 1.0 \), \( (\mu_2^u = 4, w_{11}^u = 0.75, w_{12}^u = 0.66, w_{13}^u = -3.7 \times 10^{-4}), (\mu_2^u = 5.9, w_{21}^u = 4.9 \times 10^{-3}, w_{22}^u = 0.99, w_{23}^u = -2.4 \times 10^{-6}), (u_{01} = 1.99, u_{02} = 1.99 \times 10^{-3}, u_{03} = -1.99 \). The stiffness of the problem is not altered by this variation in the parameter \( d \).

Step 5: Deng [12] notes that a homoclinic orbit exists for \( \epsilon = 0.01 \). Accordingly, we tried to increase \( \epsilon \) from \( \epsilon = 0.0093 \) (in Fig. 4.6) to \( \epsilon = 0.01 \) using the boundary conditions of Step (2a). We performed continuation with respect to \( \epsilon, \epsilon_0, (\epsilon_1, d_{11}, d_{12}, d_{13}), (\mu_1^u, w_{11}^u, w_{12}^u, w_{13}^u), (\mu_2^u, w_{21}^u, w_{22}^u, w_{23}^u), (u_{01}, u_{02}, u_{03}), \mu_1^s, \kappa \) using both Pseudo -Arclength Continuation and Natural Parameter Continuation. The continuation process did not converge.

We also attempted to use the boundary conditions of Step (3a) and perform continuation with respect to \( \epsilon, T, (\epsilon_1, d_{11}, d_{12}, d_{13}), (\mu_1^u, w_{11}^u, w_{12}^u, w_{13}^u), (\mu_2^u, w_{21}^u, w_{22}^u, w_{23}^u), (u_{01}, u_{02}, u_{03}), \mu_1^s, \kappa \), again using both Natural Parameter Continuation and Pseudo-Arclength continuation. Once more, there was no convergence.

A third attempt to perform continuation, which also met with failure was the following: At Step (2a) switch from the steering vector approximation to the eigenvector approximation on the boundary \( u(1) \) but hold \( \epsilon \) constant at \( \epsilon = 0.01 \) and solve the following problem:

\[
\begin{align*}
    u' &= Tf(u, \lambda), \\ u &= (x, y, z)
\end{align*}
\]

(4.17)

the 6 boundary conditions,

\[
\begin{align*}
    (a) \quad u(0) &= u_0 + \epsilon_0 \{ w_1^u \cos \kappa + w_2^u \sin \kappa \} \\
    (b) \quad u(1) &= u_0 + \epsilon_1 d_1
\end{align*}
\]

(4.18)

3 eigenvalue problem conditions,

\[
\begin{align*}
    f_0^u d_1 &= \mu_1^s d_1
\end{align*}
\]

(4.19)

and the normalization condition,

\[
|d_1| = 1
\]

(4.20)

We attempted to perform continuation with respect to \( \epsilon, T, (\epsilon_1, d_{11}, d_{12}, d_{13}), \mu_1^s, \kappa \) but the continuation process did not converge.

We therefore conclude that it is difficult, if not impossible to compute the homoclinic orbit for \( \epsilon = 0.01 \).
4.3 The Methods Which Failed

1. The Homotopy From Two Dimensions

The solution of problems such as the Josephson Junction [11], have been carried out using a homotopy from a known solution to a simpler problem. Since we had already obtained a homoclinic orbit for the simpler two-dimensional problem defined by the system of equations:

\[
\begin{align*}
\dot{x} &= (2 - z)a(x - 2) + (z + 2)[\alpha(x - x_0) + \beta(y - y_0)] \\
\epsilon \dot{z} &= (4 - z^2)[z + 2 - m(x + 2)] - \epsilon cz
\end{align*}
\]

we attempted to find a solution to the system,

\[
\begin{align*}
\dot{x} &= (2 - z)a(x - 2) + (z + 2)[\alpha(x - x_0) + \beta(y - y_0)] \\
\dot{y} &= \gamma \{(2 - z)[d(b - a)(x - 2) + by] + (z + 2)\{-\beta(x - x_0) + \alpha(y - y_0)\}) \\
\epsilon \dot{z} &= (4 - z^2)[z + 2 - m(x + 2)] - \epsilon cz
\end{align*}
\]

We initialized \( \gamma = 0 \), when Eq. (4.22) reduces to Eq. (4.21) and having found a homoclinic orbit for the system of ODEs in Eq. (4.21), we attempted to increase \( \gamma \) from \( \gamma = 0 \) to \( \gamma = 1 \), which would give a homoclinic orbit in three dimensions. The advantage of dealing with a two-dimensional problem first, is that the stable and unstable manifolds are one-dimensional, so we do not have to deal with unknown linear combinations of eigenvectors, which is necessary to solve the three dimensional problem. However, this approach did not meet with any success; with hindsight one can see that there is a loop in the three-dimensional orbit shown in Fig. (4.6), which does not exist in the two-dimensional orbit of Fig. (3.5), and this is probably why the homotopy fails.

2. Increasing the Singular Perturbation Parameter \( \epsilon \)

Apart from the fact, that the linear combination of eigenvectors on the two-dimensional unstable manifold, \( W_{loc}^u(u_0) \) is unknown, this problem is compounded by the fact that the system of ODEs is stiff, which makes the problem of computing homoclinic orbits even more difficult. For the two-dimensional system defined by Eq. (4.21), it was found that \( |\mu^s_i| \) could be reduced (thus making the system of ODEs less stiff) by increasing the singular perturbation parameter, \( \epsilon \). With this “insight”, we attempted to increase \( \epsilon \) using the boundary conditions of Step. (2a) and carrying out continuation with respect to \( \epsilon, T, (\epsilon_1, d_{11}, d_{12}, d_{13}), (\mu^1, w^u_{11}, w^u_{12}, w^u_{13}), (\mu^2, w^u_{21}, w^u_{22}, w^u_{23}), (u_{01}, u_{02}, u_{03}), \mu^s, \kappa \).

This method failed and the explanation is as follows: It is known theoretically from Deng [12] that a homoclinic orbit exists for \( \epsilon = 0.01 \), which means that the orbit must intersect the stable manifold \( W^s_{loc}(u_0) \) defined by the eigenvector \( w^s_i \) at the right boundary \( u(1) \). For larger values of \( \epsilon \), there is no certainty that the orbit will intersect this one dimensional stable manifold; in fact, in general the orbit will not intersect the one dimensional stable manifold. To guarantee that the orbit intersects the unstable manifold, the manifold would have to be two-dimensional which is not the case for this problem.
3. The Initial Value Problem Solver VODE

VODE is an IVP solver designed specifically to tackle systems of stiff ODEs. We intended to compute an initial orbit with VODE for the system in Eq. (4.1), and then perform continuation using AUTO, with respect to the parameters (ε, d). VODE was not able to produce the orbits, which were achieved by AUTO in Fig. (4.6). We used the data from Fig. (4.6), namely, ε = 9.3 × 10^{-3}, d = -0.2, u_{01} = 1.995, u_{02} = 3.55 × 10^{-3}, u_{03} = 1.998, w_1^u = 0.99, w_2^u = 5.21 × 10^{-4}, w_3^u = -4.92 × 10^{-4}, w_2^w = 4.92 × 10^{-3}, w_2^w = 0.99, w_3^w = -2.4 × 10^{-6}, ε_0 = 3.05 × 10^{-8}, κ = -1.89 × 10^{-6}. The results of the computation with VODE are shown in Fig. (4.8 a1–c1), and for comparison the results with AUTO are shown in Fig. (4.8 a2–c2). VODE is clearly not able to reproduce the sharp fronts, which can be computed with AUTO and worse still, the computation of y(t) is hopelessly inaccurate.

4.4 Figures.

Fig. 4.1. Initial solution showing x(t) which is constant. y(t) and z(t) are also constant.

Fig. 4.2. T = 4.3, ε_1 = 0.3, d_1 = (7.5 × 10^{-3}, -2.9 × 10^{-3}, 0.95)

Fig. 4.3a. A spurious solution plotted in the phase plane

Fig. 4.3b. Graph of y(t) showing undershooting of the y component.

Fig. 4.4. The other parameter values are d = -0.2, ε = 9.2 × 10^{-3}, T = 4.3, ε_0 = 10^{-7}, ε_1 = 0.3, κ = 5.7 × 10^{-4}, (μ_1 = -2039, d_{11} = -4.9 × 10^{-3}, d_{12} = 5.1 × 10^{-3}, d_{13} = 1.0),
(μ_2 = 4, w_1^u = 0.99, w_2^u = 0.05, w_3^u = -4.9 × 10^{-4}), (μ_2 = 5.99, w_2^u = 4.8 × 10^{-3}, w_2^w = 0.99, w_2^w = -2.3 × 10^{-6}), (u_{01} = 1.99, u_{02} = 3.3 × 10^{-3}, u_{03} = -1.99).

Fig. 4.5. The parameter values are: d = -0.2, ε = 9.3 × 10^{-3}, T = 4.3, ε_0 = 1.9 × 10^{-7}, ε_1 = 0.34, κ = -5 × 10^{-6}, (μ_1 = -2025, d_{11} = -4.9 × 10^{-3}, d_{12} = 5.1 × 10^{-3}, d_{13} = 0.99),
(μ_2 = 4, w_1^u = 0.99, w_2^u = 0.05, w_3^u = -4.9 × 10^{-4}), (μ_2 = 5.99, w_2^u = 4.9 × 10^{-3}, w_2^w = 0.99, w_2^w = -2.4 × 10^{-6}), (u_{01} = 1.99, u_{02} = 3.35 × 10^{-3}, u_{03} = -1.99).
Fig. 4.6. $e_0 = 3.7 \times 10^{-9}, \epsilon_1 = 1.0 \times 10^{-7}, \epsilon = 9.3 \times 10^{-3}, T = 5.3$. The parameter values are: $d = -0.2, \epsilon = 9.3 \times 10^{-3}, T = 5.3, \epsilon_0 = 3.7 \times 10^{-9}, \epsilon_1 = 1.1 \times 10^{-7}, \kappa = -2.7 \times 10^{-7}, (\mu_1^u = -2026, d_{11} = -4.9 \times 10^{-3}, d_{12} = 5.1 \times 10^{-3}, d_{13} = 0.99 ), (\mu_1^u = 4, w_{11}^u = 0.99, w_{12}^u = 0.05, w_{13}^u = -4.9 \times 10^{-4} ), (\mu_2^u = 5.99, w_{21}^u = 4.9 \times 10^{-3}, w_{22}^u = 0.99, w_{23}^u = -2.4 \times 10^{-6} ), (u_0 = 1.99, u_01 = 3.5 \times 10^{-3}, u_{03} = -1.99)$.

Fig. 4.7. The parameter values are: $d = -3.5, \epsilon = 9.3 \times 10^{-3}, \epsilon_0 = 4.7 \times 10^{-9}, \epsilon_1 = 1.1 \times 10^{-7}, \kappa = -1.4 \times 10^{-5}, (\mu_1^u = -2024, d_{11} = -5.3 \times 10^{-3}, d_{12} = 5.5 \times 10^{-3}, d_{13} = 1.0 ), (\mu_1^u = 4, w_{11}^u = 0.75, w_{12}^u = 0.66, w_{13}^u = -3.7 \times 10^{-4} ), (\mu_2^u = 5.9, w_{21}^u = 4.9 \times 10^{-3}, w_{22}^u = 0.99, w_{23}^u = -2.4 \times 10^{-6} ), (u_0 = 1.99, u_{02} = 1.99 \times 10^{-3}, u_{03} = -1.99)$.

Fig. 4.8 Comparison of results obtained with VODE (a1–c1) and AUTO (a2–c2). The parameter values are $\epsilon = 9.3 \times 10^{-3}, d = -0.2, u_{01} = 1.995, u_{02} = 3.55 \times 10^{-3}, u_{03} = 1.998, w_{11}^u = 0.99, w_{12}^u = 5.21 \times 10^{-4}, w_{13}^u = -4.92 \times 10^{-4}, w_{21}^u = 4.92 \times 10^{-3}, w_{22}^u = 0.99, w_{23}^u = -2.4 \times 10^{-6}, \epsilon_0 = 3.05 \times 10^{-8}, \kappa = -1.89 \times 10^{-6}$.
FIGURE 4.1
THE LABELS ARE:

1  2  3  4  5  6  7  8  9 10
11 12 13 14 15 16 17 18 19 20 21
22 23 24 25 26 27 28 29 30 31
32 33 34 35 36 37 38 39 40 41 42
43 44 45 46 47 48 49 50 51 52 53
54 55 56 57 58 59 60 61 62 63 64
65 66 67 68 69 70 71 72 73 74 75
76 77 78 79 80 81 82 83 84 85 86
87 88 89 90 91 92 93 94 95 96 97
98 99 100 101 102 103 104 105 106 107 108

ENTER NEW LABELS:

FIGURE 4.2
FIGURE 4.3a
ENTER <3D> COMMAND:

DIMENSION: 4
ENTER AXES (DEFAULT 1 2), <D> (DISPLAY), OR <EX> (EXIT)

THE LABELS ARE:

1 2 3 4 5 6 7 8 9 10
11 12 13 14 15 16 17 18 20 21
22 23 24 25 26 27 28 29 30 31
32 33 34 35 36 37 38 39 40 41
42 43 44 45 46 47 48 49 50 51
52 53 54 55 56 57 58 59 60 61
62 63 64 65 66 67 68 69 70 71
72 73 74 75 76 77 78 79 80 81
82 83 84 85 86 87 88 89 90 91

FIGURE 4.4
ENTER <3D> COMMAND:

DIMENSION: 4

ENTER AXES (DEFAULT 1 2), <D> (DISPLAY), OR <EX> (EXIT)

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FIGURE 4.5
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FIGURE 4.6
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31 32 33 34 35 36 37 38 39 40
41 42 43 44 45 46 47 48 49 50
51 52 53 54 55 56 57 58 59 60
61 62 63 64 65 66 67 68 69 70
71 72 73 74 75 76 77 78 79 80

FIGURE 4.7
FIGURE 4.8 (a1)
FIGURE 4.8 (b1)
THE LABELS ARE:

FIGURE 4.8 (c1)
FIGURE 4.8 (a2)
FIGURE 4.8 (b2)
DIMENSION : 4
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THE LABELS ARE :

1 2 3 4 5 6 7 8 9 10
11 12 13 14 15 16 17 18 20 21
22 23 24 25 26 27 28 29 30 31

FIGURE 4.8 (c2)
5. The Fluid Mechanics Problem

5.1 Parameter Assignment in AUTO

For the generic four dimensional problem, the parameter assignment is as follows:

\[ u_0 \]  \quad \text{par}(101)\text{-par}(104) \text{ left fixed point}

\[ \epsilon_0d, d_0(4) \]  \quad \text{par}(106)\text{-par}(110) \text{ left steering vector}

\[ \mu_{0i}, w_{0i} \]  \quad \text{par}(111)\text{-par}(130) \text{ 4 left eigenvalues/vectors}

\[ \epsilon_{0i} \]  \quad \text{par}(131)\text{-par}(135) \text{ 4 left eigenvector weights}

\[ u_1 \]  \quad \text{par}(151)\text{-par}(154) \text{ right fixed point}

\[ \epsilon_{1d}, d_1(4) \]  \quad \text{par}(156)\text{-par}(160) \text{ right steering vector}

\[ \mu_{1i}, w_{1i} \]  \quad \text{par}(161)\text{-par}(180) \text{ 4 right eigenvalues/vectors}

\[ \epsilon_{1i} \]  \quad \text{par}(181)\text{-par}(185) \text{ 4 right eigenvector weights}

\[ \xi_1 \]  \quad \text{par}(1)

\[ e_{11} \]  \quad \text{par}(2)

\[ e_{12} \]  \quad \text{par}(3)

\[ \xi_2 \]  \quad \text{par}(4)

\[ e_{21} \]  \quad \text{par}(5)

\[ e_{22} \]  \quad \text{par}(6)

\[ s_{34} \]  \quad \text{par}(7) \text{ sign for Eqs. (3),(4)}
5.2 Formulation of the Problem

We study this system of equations which are discussed in Eq. (2.5) in the paper by Armbruster et al [2]:

\[(a) \dot{x}_1 = x_1 x_2 + y_1 y_2 + x_1 (\xi_1 + e_{11} r_1^2 + e_{12} r_2^2) \]
\[(b) \dot{y}_1 = x_1 y_2 - y_1 x_2 + y_1 (\xi_1 + e_{11} r_1^2 + e_{12} r_2^2) \]
\[(c) \dot{x}_2 = \pm (x_1^2 - y_1^2) + x_2 (\xi_2 + e_{21} r_1^2 + e_{22} r_2^2) \]
\[(d) \dot{y}_2 = \pm 2 x_1 y_1 + y_2 (\xi_2 + e_{21} r_1^2 + e_{22} r_2^2) \]
\[r_1^2 = x_1^2 + y_1^2 \quad \text{and} \quad r_2^2 = x_2^2 + y_2^2 \]

This system of equations corresponds directly to Eq.(28) of Aubry [1]:

\[v_2 = c_{4,-2} (v_4 v_2 + w_4 w_2) + v_2 (a_2 + d_{22} r_2^2 + d_{24} r_2^4) \]
\[w_2 = c_{4,-2} (v_2 w_4 - v_4 w_2) + w_2 (a_2 + d_{22} r_2^2 + d_{24} r_2^4) \]
\[w_4 = c_{2,2} (v_2^2 - w_2^2) + v_4 (a_4 + d_{42} r_2^2 + d_{44} r_2^4) \]
\[r_2^2 = v_2^2 + w_2^2 \quad \text{and} \quad r_4^2 = v_4^2 + w_4^2 \]

The systems in Eq. (5.1) and Eq. (5.2) are obtained from the Navier-Stokes equations [1]. The fluctuating component of the velocity is expanded as a Fourier series in the spanwise and streamwise directions. A Galerkin projection is applied to convert the system of PDEs into a system of ODEs. The series is then truncated to retain only the first few terms in the Fourier expansion because the Galerkin approximation minimizes the error due to truncation. The important parameters in the Armbruster system are \(\xi_1\) and \(\xi_2\), which correspond to the parameters \(a_2\) and \(a_4\) of the Aubry system. \(a_2\) and \(a_4\) are related to the Heisenberg parameters \(\alpha_1\) and \(\alpha_2\) and the Reynolds’ number \(Re_T\) by the equation:

\[a_k = a_k^1 + (1 + \alpha_1 / Re_T) a_k^2 \]
\[c_{k',k-k'} = c_{k',k-k'}^1 + \alpha_2 c_{k',k-k'}^2 \]

The Heisenberg parameters \(\alpha_1\) and \(\alpha_2\) may be adjusted upward and downward to simulate greater and smaller energy losses to the unresolved modes, corresponding to the presence of a greater or smaller intensity of smaller-scale turbulence in the neighborhood of the wall. This might correspond to the environment just before or just after a bursting event which produces a large burst of small scale turbulence which is then diffused to the outer part of the layer.

We wish to investigate the dynamical behavior of the system defined by Eq. (5.1). The initial value used was directed along \(w_0^4\) with \(e_0 = 10^{-7}\) as follows: \(u(t) = u_0 + e_0 w_0\). Continuation was carried out with respect to the period which was initially set at \(T = 0.01\) and increased till \(T = 130\).
The initial values at the left fixed point $u_0$ were the following:

$$f_u(u_0, \lambda) = \begin{pmatrix}
0.18 & 0 & 0 & 0 \\
0 & -0.34 & 0 & 0 \\
0 & 0 & -0.40 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}$$

\(w_u^u = (1, 0, 0, 0)\)

\(\xi_0^u = 0.18\)

\(u_0 = (0, 0, \pm(-\mu_2/c_{22})^{1/2}, 0)\)

### 5.3 Computational Results

We use the following notation:

- $u_0 = (u_{01}, u_{02}, u_{03}, u_{04})$: Fixed Point near left boundary
- $u_1 = (u_{11}, u_{12}, u_{13}, u_{14})$: Fixed Point near right boundary
- $w_u^u$: Eigenvector defining unstable manifold at $u_0$
- $\mu_0^u$: Eigenvalue corresponding to $w_u^u$
- $d_1 = (d_{11}, d_{12}, d_{13}, d_{14})$: Normalized steering vector components connecting $u_1$ and $u(1)$
- $\epsilon_0$: Distance between $u_0$ and $u(0)$
- $\epsilon_1$: Distance between $u_1$ and $u(1)$

For the system of equations defined by Eq. (5.1) with the negative sign used in Eq. (5.1 c-d), we attempt to generate Fig. (5c) in the paper by Armbruster [2] for which we used the parameter values: $\epsilon_{11} = -4, \epsilon_{12} = -1, \epsilon_{21} = -1, \epsilon_{22} = -2, \xi_1 = -0.03, \xi_2 = 0.2$.

The unstable manifold $W_{loc}^u(u_0)$ at $u_0$ is one dimensional and its direction is defined by the eigenvector $w_u^u$. The stable manifold $W_{loc}^s(u_1)$ at $u_1$ is two dimensional and since it is difficult to determine the linear combination of eigenvectors which determine its direction we use the steering vector $d_1$ at this boundary.

**Step 1.** Initialize the period $T$ by a "small" number, such as 0.01, and the "distance" $\epsilon_0$ by another "small" number, such as $10^{-7}$. Given $u_0$ and $w_u^u$, with $|w_u^u| = 1$ initialize the solution by a constant:

\[(5.5)\]

\[u(t) = u_0 + \epsilon_0 w_u^u, \ 0 < t < 1.\]

and set the tolerances $\epsilon_u = \epsilon_\lambda = 10^{-8}$ and set the number of subintervals and collocation points to $NTST = 25$ and $NCOL = 4$ respectively. Eq. (5.6) and Eq. (5.7) represent a total of 9 boundary conditions. We perform continuation with respect to $(T, \epsilon_1, d_{11}, d_{12}, d_{13}, d_{14})$. We have now reached Fig. (5.1), where $(T = 168, \epsilon_1 = 7.5 \times 10^{-9}, d_{11} = 0.04, d_{12} = 0, d_{13} = 0.99, d_{14} = 0 )$.
Step 2 We will now attempt to repeat the results of Fig. (5e) in Armbruster [2], where \((\xi_1 = 0.135, \xi_2 = 0.2)\). For these parameter values, modulated travelling waves coexist with the heteroclinic orbit. Moreover it is precisely at these parameter values that a bifurcation occurs from the 2-dimensional heteroclinic orbit shown in Fig. (5.1) where \((\xi_1 = -0.03, \xi_2 = 0.2)\) to a full 4-dimensional heteroclinic orbit. To reach \((\xi_1 = 0.135, \xi_2 = 0.2)\) we follow a multistep continuation procedure, where the problem is formulated as follows:

\[
(5.6) \quad u'(t) - T f(u(t), \lambda) = 0, \quad 0 < t < 1,
\]

\[
(5.7) \quad \begin{align*}
& (a) \quad f(u_0, \lambda) = 0 \\
& (b) \quad f(u_1, \lambda) = 0,
\end{align*}
\]

\[
(5.8) \quad \begin{align*}
& a) \quad u(0) = u_0 + \epsilon_0 w_0^n, \\
& b) \quad u(1) = u_1 + \epsilon_1 d_1, \quad d_1 \in \mathbb{R}^n
\end{align*}
\]

\[
(5.9) \quad f_u(u_0, \lambda) w_0^n = \mu_0^n w_0^n, \quad w_0^n \in \mathbb{R}^n, \quad \mu_0^n \in \mathbb{R},
\]

\[
(5.10) \quad \begin{align*}
& (a) \quad |d_1| = 1 \\
& (b) \quad |w_0^n| = 1,
\end{align*}
\]

\[
(5.11) \quad \int_0^1 (f(u(t), \lambda) - f(q(t), \lambda^0)) \cdot f_u(u(t), \lambda) f(u(t), \lambda) dt = 0.
\]

There are 22 boundary conditions plus an Integral Condition. Continuation is performed with respect to the 20 parameters.

**Step (2a):** Perform continuation with respect to \((\xi_1, \xi_2, T), (u_{01}, u_{02}, u_{03}, u_{04}), (u_{11}, u_{12}, u_{13}, u_{14}), (d_{11}, d_{12}, d_{13}, d_{14}), (\mu_0^n, w_{01}^n, w_{02}^n, w_{03}^n, w_{04}^n)\). The continuation process fails to converge at the terminal values of \((\xi_1 = -3.9 \times 10^{-3}, \xi_2 = 0.198), (T = 124, \epsilon_0 = 10^{-7}, \epsilon_1 = 10^{-6})\), \((u_{01} = 0, u_{02} = 0, u_{03} = 0.315, u_{04} = 0), (u_{11} = 0, u_{12} = 0, u_{13} = -0.315, u_{14} = 0), (d_{11} = 0.14, d_{12} = -1.4 \times 10^{-8}, d_{13} = 0.98, d_{14} = 0.065)\), \((\mu_0^n = 0.2, w_{01}^n = 1, w_{02}^n = 0, w_{03}^n = 0, w_{04}^n = 0)\).

**Step (2b):** Using these terminal values, perform continuation with respect to \((\xi_1, \xi_2, \epsilon_0), (u_{01}, u_{02}, u_{03}, u_{04}), (u_{11}, u_{12}, u_{13}, u_{14}), (d_{11}, d_{12}, d_{13}, d_{14}), (\mu_0^n, w_{01}^n, w_{02}^n, w_{03}^n, w_{04}^n)\).

The continuation fails to converge at the terminal values \((\xi_1 = 0.1, \xi_2 = 0.21), (T = 124, \epsilon_0 = 8.5 \times 10^{-9}, \epsilon_1 = 10^{-6})\), \((u_{01} = 0, u_{02} = 0, u_{03} = 0.323, u_{04} = 0), (u_{11} =

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0, \( u_{12} = 0, u_{13} = -0.323, u_{14} = 0 \), (\( d_{11} = 0.79, d_{12} = -6.7 \times 10^{-7}, d_{13} = 0.019, d_{14} = 0.060 \)), (\( \mu^w_0 = 0.326, w_{01}^w = 1, w_{02}^w = 0, w_{03}^w = 0, w_{04}^w = 0 \)).

**Step (2c):** Using these terminal values perform continuation with respect to 
(\( \xi_1, \xi_2, \xi_3 \), \( u_{01}, u_{02}, u_{03}, u_{04} \)), (\( u_{11}, u_{12}, u_{13}, u_{14} \)), (\( d_{11}, d_{12}, d_{13}, d_{14} \)), (\( \mu^w_0, w_{01}^w, w_{02}^w, w_{03}^w, w_{04}^w \)). Continuation proceeds till we reach Fig. (5.2) where (\( \xi_1 = 0.138, \xi_2 = 0.21 \)), (\( T = 124, \epsilon_0 = 8.5 \times 10^{-9}, \epsilon_1 = 2.3 \times 10^{-6} \)), (\( u_{01} = 0, u_{02} = 0, u_{03} = 0.323, u_{04} = 0 \)), (\( u_{11} = 0, u_{12} = 0, u_{13} = -0.323, u_{14} = 0 \)), (\( d_{11} = 0.96, d_{12} = -8.1 \times 10^{-7}, d_{13} = 4.5 \times 10^{-3}, d_{14} = 0.268 \)), (\( \mu^w_0 = 0.326, w_{01}^w = 1, w_{02}^w = 0, w_{03}^w = 0, w_{04}^w = 0 \)).

**Step 3:** We will also attempt to reproduce the bifurcation diagram for the branch of heteroclinic orbits, shown in Fig. 3 in Armbruster [2]. Using the same set of boundary conditions as in Step 2, increase the number of subintervals to \( NTST = 55 \). Using the initial values from Fig. (5.1), perform continuation with respect to (\( \xi_1, \xi_2, T \)), (\( u_{01}, u_{02}, u_{03}, u_{04} \)), (\( u_{11}, u_{12}, u_{13}, u_{14} \)), (\( d_{11}, d_{12}, d_{13}, d_{14} \)), (\( \mu^w_0, w_{01}^w, w_{02}^w, w_{03}^w, w_{04}^w \)). The bifurcation diagram of (\( \xi_1, \xi_2 \)) is shown in Fig. (5.3), where the initial values are (\( \xi_1 = -0.03, \xi_2 = 0.2 \)) and the final values are (\( \xi_1 = -0.036, \xi_2 = 0.09 \)). The entire bifurcation diagram in Fig. (5.3) has a number of bifurcating branches. We have traced out only one branch. This may account for the fact that our results do not match those of Armbruster [2].

**5.4 Figures**

**Fig. 5.1** \( T = 168, \epsilon_1 = 7.5 \times 10^{-9}, d_{11} = 0.04, d_{12} = 0, d_{13} = 0.99, d_{14} = 0 \).

**Fig. 5.2** (\( \xi_1 = 0.138, \xi_2 = 0.21 \)), \( T = 124, \epsilon_0 = 8.5 \times 10^{-9}, \epsilon_1 = 2.3 \times 10^{-6} \)), (\( u_{01} = 0, u_{02} = 0, u_{03} = 0.323, u_{04} = 0 \)), (\( u_{11} = 0, u_{12} = 0, u_{13} = -0.323, u_{14} = 0 \)), (\( d_{11} = 0.96, d_{12} = -8.1 \times 10^{-7}, d_{13} = 4.5 \times 10^{-3}, d_{14} = 0.268 \)), (\( \mu^w_0 = 0.326, w_{01}^w = 1, w_{02}^w = 0, w_{03}^w = 0, w_{04}^w = 0 \)).

**Fig. 5.3** The initial values are (\( \xi_1 = -0.03, \xi_2 = 0.2 \)) and the final values are (\( \xi_1 = -0.036, \xi_2 = 0.09 \)).
FIGURE 5.1
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FIGURE 5.1 (Cont.)
FIGURE 5.1 (Con't.)
FIGURE 5.2
FIGURE 5.2 (Con't.)
FIGURE 5.2 (Con't.)
FIGURE 5.2 (Con't.)
FIGURE 5.2 (Con't.)
6. Conclusions and Recommendations.

*Homoclinic and heteroclinic* orbits are orbits of an infinite period connecting two fixed points of an associated system of autonomous ordinary differential equations. Homoclinic orbits have been shown to play a fundamental role in phenomena such as bursting in biology, chaotic vibrations of structures, chaotic oscillations in chemical reactions, etc. Heteroclinic orbits are equally important in the understanding of the global behavior of dynamical systems, turbulence, and also in the study of wave phenomena in nonlinear parabolic partial differential equations.

In earlier papers Doedel and Friedman have developed an accurate, robust, and systematic numerical method and derived error estimates for the computation of branches of homoclinic and heteroclinic orbits. The idea of the method is to reduce a boundary value problem on the real line to a boundary value problem on a finite interval by using a local (linear or higher order) approximation of the stable and unstable manifolds and then study the reduced problem using a continuation software package such as AUTO.

Theoretical analysis of homoclinic and heteroclinic orbits is often conducted in the context of singular perturbation problems. In this paper we have refined and extended earlier algorithms of Doedel and Friedman using 2 model singular perturbation problems and a turbulent fluid boundary layers in the wall region problem. We have thus considerably extended the range of applicability of our algorithms.
References


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Prepared for:
NASA (sp out)
Marshall Space Flight Center

I have reviewed this report, dated 10 September 1972, and the report contains no classified information.

Principal Investigator
# Title
Accurate Computation and Continuation of Homoclinic and Heteroclinic Orbits for Singular Perturbation Problems

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## Abstract
In earlier papers (see [11] and references therein) Doedel and the authors have developed a numerical method and derived error estimates for the computation of branches of heteroclinic orbits for a system of autonomous ordinary differential equations in $\mathbb{R}^3$. The idea of the method is to reduce a boundary value problem on the real line to a boundary value problem on a finite interval by using a local (linear or higher order) approximation of the stable and unstable manifolds. A practical limitation for the computation of homoclinic and heteroclinic orbits has been the difficulty in obtaining starting orbits. Typically these were obtained from a closed form solution or via a homotopy from a known solution. Here we consider extensions of our algorithm which allow us to obtain starting orbits on the continuation branch in a more systematic way as well as make the continuation algorithm more flexible. In applications we use the continuation software package AUTO in combination with some initial value software. The examples considered include computation of homoclinic orbits in a singular perturbation problem and in a turbulent fluid boundary layer in the wall region problem.

## Subject Terms
Heteroclinic Orbits, Computation and Continuation, Singular Perturbation