

IBM Research Report

Multiparameter Parallel Search Branch Switching

Michael E. Henderson
IBM Research Division
Thomas J. Watson Research Center
P.O. Box 218
Yorktown Heights, NY 10598



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MULTIPARAMETER PARALLEL SEARCH BRANCH SWITCHING

MICHAEL E. HENDERSON
IBM RESEARCH DIVISION
T. J. WATSON RESEARCH CENTER
YORKTOWN HEIGHTS, NY 10598
MHENDER@WATSON.IBM.COM

Abstract. A continuation method (sometimes called path following) is a way to compute solution curves of a nonlinear system of equations with a parameter. We derive a simple algorithm for branch switching at bifurcation points for multiple parameter continuation, where surfaces bifurcate along a singular curves on a surface. It is a generalization of the parallel search technique used in the continuation code AUTO, and avoids the need for second derivatives and a full analysis of the bifurcation point.

The one parameter case is special. While the generalization is not difficult, it is non-trivial, and the geometric interpretation may be of some interest. An additional tangent calculation at a point near the singular point is used to estimate the tangent to the singular set.

1. Background and basic result. A continuation method (sometimes called path following) is a way to compute solution curves of a nonlinear system of equations with a parameter. For an introduction to these methods see, for example, the books by Allgower and Georg [1], Garcia and Zangwill [6] and more recently Govaerts [7], Beyn et al. [3], and papers by Doedel [5] and Seydel [14].

In [9] the author described a generalization of these methods to problems with more than one parameter, where the solution manifolds are surfaces instead of curves. One practical issue that was not addressed there is how to generalize the second-derivative-free parallel search branch switching algorithm that is used in codes like AUTO, [11], [10]. The one parameter case is special. While the generalization is not difficult, it is non-trivial, and the geometric interpretation may be of some interest.

Suppose Γ_0 is a regular connected component of the solution manifold of

$$\mathbf{F}(\mathbf{u}) = 0, \quad \mathbf{u} \in \mathbb{R}^n \quad \mathbf{F} : \mathbb{R}^n \rightarrow \mathbb{R}^{n-k}$$

containing the initial point \mathbf{u}_0 and restricted to some computational domain $\Omega \subset \mathbb{R}^n$. That is, a point \mathbf{v} is in Γ_0 if there is a continuous curve $\mathbf{u}(s)$, $s \in [0, 1]$, of regular solutions of $\mathbf{F} = 0$ connecting \mathbf{v} to \mathbf{u}_0 through Ω (see Figure 1.1)

$$\begin{aligned} \mathbf{F}(\mathbf{u}(s)) &= 0, & \mathbf{u}(s) &\subset \Omega, \\ \text{rank}(\mathbf{F}_{\mathbf{u}}(\mathbf{u}(s))) &= n - k, \\ \mathbf{u}(0) &= \mathbf{u}_0, & \mathbf{u}(1) &= \mathbf{v}. \end{aligned}$$

If \mathbf{F} is smooth, Γ_0 is a k dimensional manifold with a boundary, and the boundary is made up of $(k - 1)$ dimensional manifolds (again with boundaries) which either lie on $\delta\Omega$, or are such that the Jacobian $\mathbf{F}_{\mathbf{u}}$ is of rank $n - k - 1$.

Consider a point \mathbf{u}^* on the singular boundary of Γ_0 (see Figure 1.2). This point can be found by monitoring an indicator function $\chi(\mathbf{u})$, which changes sign or jumps when evaluated for points on opposite sides of a singular curve. (See [3] for a description of indicator functions for various bifurcations.) Bisection or a root finding algorithm may then be used to locate \mathbf{u}^* in the interval $[\mathbf{u}_a, \mathbf{u}_b]$ where the indicator function changes. The aim of branch switching is to find points near \mathbf{u}^* that are interior to the other regular connected components containing \mathbf{u}^* (Figure 1.3).

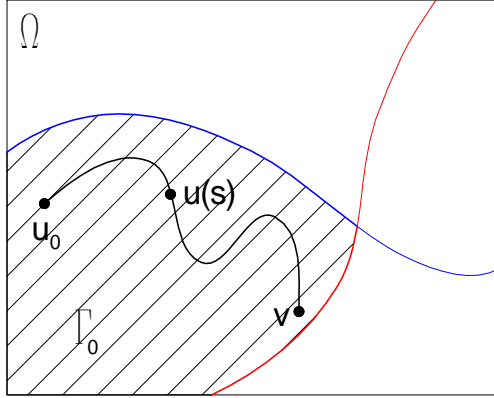


FIG. 1.1. A regular connected component Γ_0 of $\mathbf{F} = 0$ in Ω . For every point \mathbf{v} in Γ_0 there is a path $\mathbf{u}(s)$ of regular solutions connecting it to \mathbf{u}_0 .

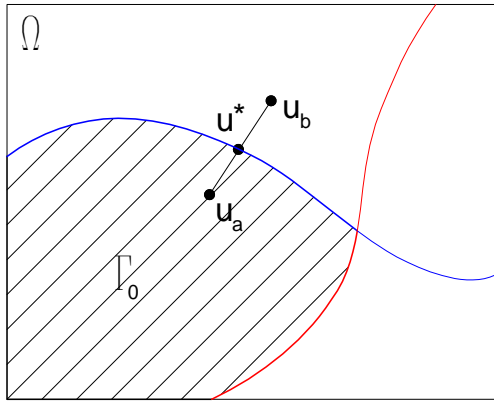


FIG. 1.2. The singular boundary of a regular connected component. Points on this boundary, like \mathbf{u}^* , are found by monitoring a test function which changes between points on opposite sides of the boundary (\mathbf{u}_a and \mathbf{u}_b). Bisection or a root finding algorithm may be used to locate \mathbf{u}^* .

1.1. The geometry of the solution manifold near a singular point. The tangent space of Γ_0 at the singular boundary point can be found by interpolation between the tangent spaces at \mathbf{u}_a and \mathbf{u}_b (which are regular points and have unique tangent spaces). We can therefore find an orthonormal basis $\{\phi_0, \dots, \phi_{k-1}\}$ for the k -dimensional tangent space of Γ_0 at \mathbf{u}^*

$$\begin{aligned} \mathbf{F}_{\mathbf{u}}(\mathbf{u}^*)\phi_i &= 0 \\ \phi_i^T \phi_j &= \delta_{ij} \end{aligned}$$

If \mathbf{u}^* is interior to the singular boundary, the rank of $\mathbf{F}_{\mathbf{u}}(\mathbf{u}^*)$ will be $n - k - 1$, and so there is a right null vector $\phi_k \in \mathbb{R}^n$, and left null vector $\psi \in \mathbb{R}^{n-k}$ of the augmented

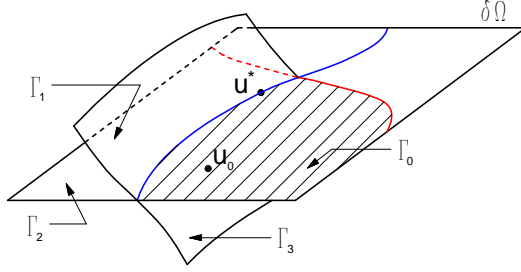


FIG. 1.3. The regular connected components sharing a point \mathbf{u}^* on their singular boundaries.

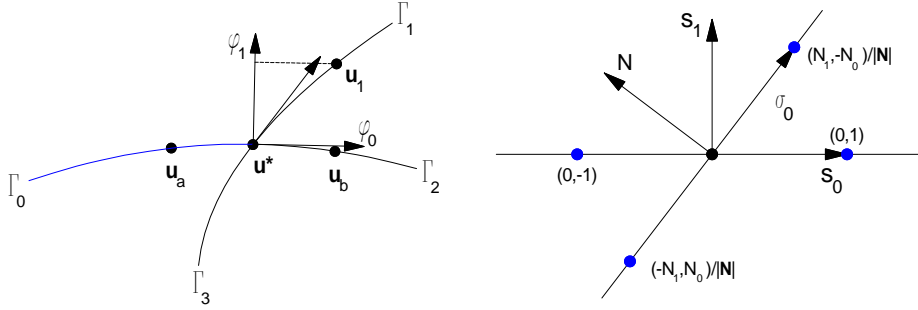


FIG. 1.4. (left) The parallel search branch switching algorithm used in AUTO. A bifurcation point \mathbf{u}^* is located between \mathbf{u}_a and \mathbf{u}_b , and the null vector of the augmented Jacobian ϕ_1 is used as a tangent for the next step. (right) A sketch of the corresponding s -space, showing the four roots of the ABE.

Jacobian

$$\begin{aligned} \mathbf{F}_{\mathbf{u}}(\mathbf{u}^*)\phi_k &= 0 & \psi^T \mathbf{F}_{\mathbf{u}}(\mathbf{u}^*) &= 0 \\ \phi_i^T \phi_k &= 0 \quad (i \neq k) \\ \phi_k^T \phi_k &= 1 & \psi^T \psi &= 1 \end{aligned}$$

To study the geometry of the bifurcation we use a Lyapunov-Schmidt decomposition. Let

$$\mathbf{u} = \mathbf{u}^* + \sum_{i=0}^k \phi_i s^i + \eta, \quad \phi_i^T \eta = 0,$$

and consider first the projection of \mathbf{F} onto the range of the Jacobian

$$(I - \psi\psi^*)\mathbf{F}(\mathbf{u}^* + \sum_{i=0}^k \phi_i s^i + \eta) = 0$$

$$\phi_i^T \eta = 0$$

as a system for η . The Jacobian at the solution $s^i = 0, \eta = 0$ is nonsingular, so using the Implicit Function Theorem (IFT) there is a unique function $\eta(s^0, \dots, s^k)$ which satisfies the projected equations in a neighborhood of $s^i = 0$. At $s^i = 0$ we have

$$\begin{aligned}\eta &= 0, & \eta_{,s^i} &= 0 \\ (I - \psi\psi^*) (\mathbf{F}_{\mathbf{u}}\eta_{,s^i,s^j} + \mathbf{F}_{\mathbf{uu}}\phi_i\phi_j) &= 0 \\ \phi_l^T \eta_{,s^i,s^j} &= 0\end{aligned}$$

(Similar equations can be written for the higher derivatives of η by repeated differentiation.)

To satisfy $\mathbf{F} = 0$ one further scalar equation must be satisfied (the Bifurcation Equation Eq. (1.1))

$$(1.1) \quad \psi^* \mathbf{F}(\mathbf{u}^* + \sum_{i=0}^k \phi_i s^i + \eta(s^0, \dots, s^k)) = 0.$$

The linearization of this is zero at $\mathbf{s} = 0$, and we can remove this so that the IFT can be used by introducing a small number ϵ –

$$\begin{aligned}\frac{1}{\epsilon^2} \psi^* \mathbf{F}(\mathbf{u}^* + \epsilon \sum_{i=0}^k \phi_i s^i + \eta(\epsilon s^0, \dots, \epsilon s^k)) &= 0, \\ s^i s^i &= 1.\end{aligned}$$

A Taylor series (in ϵ) of this begins:

$$\frac{1}{\epsilon^2} \psi^* \mathbf{F} = \sum_{i,j} \psi^T \mathbf{F}_{\mathbf{uu}} \phi_i \phi_j s^i s^j + \epsilon \sum_{i,j,l} (\psi^T \mathbf{F}_{\mathbf{uuu}} \phi_i \phi_j \phi_l s^i s^j s^l + \psi^T \mathbf{F}_{\mathbf{uu}} \phi_l \eta_{,s^i,s^j} s^l) + \dots$$

If the Algebraic Bifurcation Equation (ABE) Eq. (1.2)

$$(1.2) \quad \psi^T \mathbf{F}_{\mathbf{uu}} \phi_i \phi_j s^i s^j = 0$$

is satisfied and the first order term is non-zero

$$\psi^T \mathbf{F}_{\mathbf{uuu}} \phi_i \phi_j \phi_l s^i s^j s^l + \psi^T \mathbf{F}_{\mathbf{uu}} \phi_l \eta_{,s^i,s^j} s^l \neq 0.$$

Using the IFT, a set of functions $s^i(\epsilon)$ with $s^i(0) = s^i$ exists in a neighborhood of $\epsilon = 0$. Each solution of the ABE therefore corresponds to a curve (parameterized by ϵ) on the solution surface through \mathbf{u}^* . Varying the s^i subject to the ABE traces out the surface.

We know one set of solutions – any vector s with $s^k = 0$. (This is because we chose the first k null vectors to be a basis for the tangent space of Γ_0 .) The ABE is therefore of the form

$$s^k \left(\sum_{i=0}^k \psi^T \mathbf{F}_{\mathbf{uu}} \phi_i \phi_k s^i \right) = 0, \quad \text{or} \quad s^k \left(\sum_{i=0}^k N_i s^i \right) = 0.$$

Therefore $\mathbf{N} \in \mathbb{R}^{k+1}$ is orthogonal to the bifurcating branch, and $N_i = \psi^T \mathbf{F}_{\mathbf{u}\mathbf{u}} \phi_i \phi_k$. The tangent space of the singular boundary is

$$s^k = 0, \quad \sum_{i=0}^k N_i s^i = 0$$

Let $\{\sigma_0, \dots, \sigma_{k-2}\}$ be an orthonormal basis for this $k-1$ dimensional tangent space. The tangent space to the bifurcating sheet includes the additional vector $\sigma_{k-1} = (N_k N_0, \dots, N_k N_{k-1}, -\sum_0^{k-1} N_i N_i)$. This is orthogonal to both \mathbf{N} and the other σ_i . (It is not normalized.)

1.2. Special case: $k = 1$. When $k = 1$ the singular set is a point (see Figure 1.4). We have

$$(N_0, N_1) = (\psi^T \mathbf{F}_{\mathbf{u}\mathbf{u}} \phi_0 \phi_1, \psi^T \mathbf{F}_{\mathbf{u}\mathbf{u}} \phi_1 \phi_1),$$

and the tangent (not normalized) of the bifurcating branch in \mathbf{s} -space is

$$\sigma_{k-1} = N_0(N_1, -N_0)$$

1.3. Special case: $k = 2$. The vector (s^0, s^1, s^2) gives a point in the $k+1 = 3$ dimensional null space of $\mathbf{F}_{\mathbf{u}}(\mathbf{u}^*)$ (in the basis ϕ_0, ϕ_1, ϕ_2) (Figure 1.5). We have

$$(N_0, N_1, N_2) = (\psi^T \mathbf{F}_{\mathbf{u}\mathbf{u}} \phi_0 \phi_2, \psi^T \mathbf{F}_{\mathbf{u}\mathbf{u}} \phi_1 \phi_2, \psi^T \mathbf{F}_{\mathbf{u}\mathbf{u}} \phi_2 \phi_2).$$

The branch corresponding to Γ_0 (and Γ_2) is $s^2 = 0$

$$\begin{aligned} \mathbf{u}^* + \epsilon (\phi_0 s^0 + \phi_1 s^1) + \eta (\epsilon s^0, \epsilon s^1, 0), \\ s^0 s^0 + s^1 s^1 = 1 \end{aligned}$$

The other branches (Γ_1 and Γ_3) are

$$\begin{aligned} \mathbf{u}^* + \epsilon (\phi_0 s^0 + \phi_1 s^1 + \phi_2 s^2) + \eta (\epsilon s^0, \epsilon s^1, \epsilon s^2), \\ N_0 s^0 + N_1 s^1 + N_2 s^2 = 0 \\ s^0 s^0 + s^1 s^1 + s^2 s^2 = 1 \end{aligned}$$

See Figure 1.5. The tangent to the singular set is, in \mathbf{s} -space and \mathbb{R}^n

$$\sigma_0 = (-N_1, N_0, 0) \quad \leftrightarrow \quad -N_1 \phi_1 + N_0 \phi_0$$

and the tangent vector (not normalized, and in \mathbf{s} -space) to the bifurcating branch orthogonal to the singular set is

$$\sigma_1 = (N_0 N_2, N_1 N_2, -N_0 N_0 - N_1 N_1)$$

1.4. Parallel search branch switching. These quantities can be computed, and the tangent to the bifurcating components found directly. However, in many instances the second derivatives are not available, and we need a branch switching algorithm which does not assume they are.

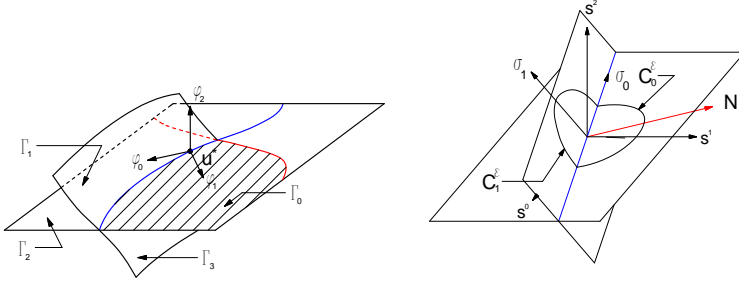


FIG. 1.5. (left) The basis for the right null space of $\mathbf{F}_{\mathbf{u}}(\mathbf{u}^*)$. The first two $(k-1)$ basis vectors lie in the tangent plane of Γ_0 (and Γ_1). The third is orthogonal to the first two. (right) Solutions to the ABE's in s -space. Circle C_0 is $s^2 = 0$, $s^0 s^0 + s^1 s^1 = 1$. Circle C_1 lies in the plane $N \cdot s = 0$, where $N = (\psi^T \mathbf{F}_{\mathbf{u}\mathbf{u}} \phi_0 \phi_2, \psi^T \mathbf{F}_{\mathbf{u}\mathbf{u}} \phi_1 \phi_2, \psi^T \mathbf{F}_{\mathbf{u}\mathbf{u}} \phi_2 \phi_2)$. The singular set is $N \cdot s = 0$, $s^k = 0$.

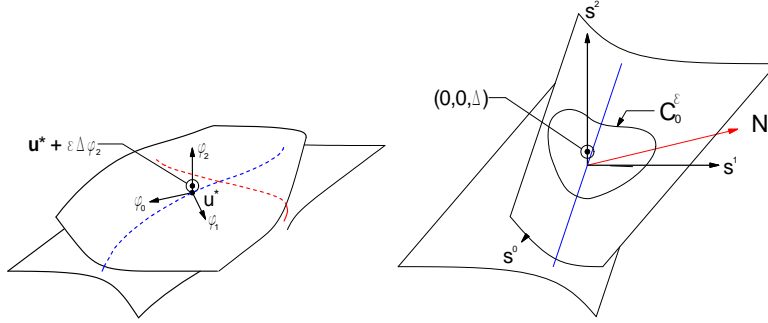


FIG. 1.6. (left) The perturbed surface $\mathbf{F}(\mathbf{u}) = \mathbf{F}(\mathbf{u}^* + \epsilon \Delta \phi_k)$. (right) The same surface in the s -space defined by the unperturbed problem.

The goal is to find a point on the bifurcating component which can be used as an initial point to compute the component. To project a point \mathbf{v} onto a regular component, a system of the form

$$\begin{aligned} \mathbf{F}(\mathbf{u}) &= 0 \\ \tilde{\Phi}^T(\mathbf{u} - \mathbf{v}) &= 0 \end{aligned}$$

is used. As long as the projection of the k vectors $\tilde{\Phi}$ (the columns) onto the null space of the Jacobian at \mathbf{u} spans the null space this is a non-singular system. As the name parallel search implies, we choose $\tilde{\Phi}$ orthogonal to the tangent to Γ_0 . The condition that the augmented Jacobian be non-singular is that the bifurcation be transverse to Γ_0 .

For $k = 1$, ϕ_1 has a non-zero projection onto the tangent to the bifurcating curve $N_1 \phi_0 - N_0 \phi_1$ if $N_0 \neq 0$ (the non-transverse case). So a point on the bifurcating branch may be found by solving

$$\begin{aligned} \mathbf{F}(\mathbf{u}) &= 0 \\ \phi_1^T(\mathbf{u} - (\mathbf{u}^* + \Delta s \phi_1)) &= 0 \end{aligned}$$

This is the technique used in AUTO (described in [3] and [11]).

For $k > 1$ we need to find a k dimensional subspace whose projection onto the tangent space of the bifurcating sheet spans that tangent space. For $k = 1$ we project orthogonal to ϕ_k . This defines a $k - 1$ dimensional curve on the bifurcating sheet, and so if $k \neq 1$ we need additional constraints to define a unique point on the bifurcating sheet. The tangent to the singular set lies in both tangent spaces, and we need to project orthogonal to that as well.

To estimate the tangent to the singular set we use a perturbation

$$\tilde{\mathbf{F}}(\mathbf{u}) = \mathbf{F}(\mathbf{u}) - \mathbf{F}(\mathbf{u}^* + \epsilon\Delta\phi_k).$$

For this (as before $N_i = \psi^* \mathbf{F}_{\mathbf{u}\mathbf{u}} \phi_i \phi_k$)

$$\frac{1}{\epsilon^2} \psi^T \tilde{\mathbf{F}} = \sum_{i=0}^k N_i s^i s^k - N_k \Delta^2 + O(\epsilon).$$

In s -space solutions of this perturbed equation are a pair of hyperbolic sheets which asymptote to the solutions of the unperturbed equation.

Suppose σ is any vector in the tangent space of the singular set. That is

$$\sum_{i=0}^k N_i \sigma^i = 0 \quad \sigma^k = 0$$

By construction, we know one point on the perturbed surface, $\mathbf{u}^* + \epsilon\phi_k$, which corresponds to the point $(0, \dots, 0, \Delta)$ in the s -space since it is a solution of

$$\sum_{i=0}^k N_i s^i s^k = \Delta^2 N_k.$$

This equation is invariant to a shift in the σ direction, so σ lies in the tangent space of the perturbed system at the known point $(0, \dots, 0, \Delta)$. This gives us a way to compute the tangent space of the singular set: it is the common $k - 1$ dimensional subspace of the tangent to Γ_0 and the tangent of the perturbed system (the null space of $\mathbf{f}_{\mathbf{u}}(\mathbf{u}^* + \epsilon\phi_k)$).

2. Statement of the algorithm.

Detection – Locate a pair of points \mathbf{u}_a and \mathbf{u}_b on $\mathbf{F} = 0$ such that $\chi(\mathbf{u}_a) \neq \chi(\mathbf{u}_b)$.

Location – Using bisection, or a root finding method locate the point \mathbf{u}^* on $\mathbf{F} = 0$ in the interval at which $\chi(\mathbf{u})$ changes. Use the tangent spaces at \mathbf{u}_a and \mathbf{u}_b to interpolate $(\phi_0, \dots, \phi_{k-1})$, an orthonormal approximation to a basis for the tangent space of Γ_0 at \mathbf{u}^* .

Branch Switching –

1. Find the right null vector ϕ_k , $\phi_k^T \phi_k = 1$

$$\mathbf{F}_{\mathbf{u}}(\mathbf{u}^*) \phi_k = 0$$

$$\phi_i^T \phi_k = 0, \quad i = 0, \dots, k - 1$$

2. Find an orthonormal basis $\tilde{\Phi}$ of the k -dimensional null space of

$$\mathbf{F}_{\mathbf{u}}(\mathbf{u}^* + \epsilon\Delta\phi_k) \tilde{\phi}_i = 0$$

$$\tilde{\phi}_i^T \tilde{\phi}_j = \delta_{ij}$$

3. Find an orthonormal basis $\{\sigma_0, \dots, \sigma_{k-2}\}$ for the common subspace of Φ and $\tilde{\Phi}$. Since ϕ_k is orthogonal to Φ this is the subspace $\phi_k^T \tilde{\Phi} = 0$, so the Gram-Schmidt algorithm can be used on the set of $k+1$ vector $\{\phi_k, \tilde{\phi}_0, \dots, \tilde{\phi}_{k-1}\}$ to find the subspace (the first will be ϕ_k , and the last will be zero the ones in between are the σ_i).
4. Find points on the bifurcating sheets by solving

$$\mathbf{F}(\mathbf{u}) = 0$$

$$\sigma_i^T (\mathbf{u} - (\mathbf{u}^* + \Delta s \phi_k)) = 0, \quad i = 0, \dots, k-2$$

$$\phi_k^T (\mathbf{u} - (\mathbf{u}^* + \Delta s \phi_k)) = 0$$

With $\Delta s > 0$ we get a point on Γ_1 , and $\Delta s < 0$ gives a point on Γ_3 . For the point on Γ_2 we can use \mathbf{u}_b , which was found in the detection step.

Notes:

- Δ controls the shape of the hyperbola in s -space, and ϵ is small relative to the norm of \mathbf{u}^* . Therefore $\epsilon\Delta$ should be something like $10^{-3}|\mathbf{u}^*|$.
- There is a technique, described in [1] which perturbs the problem in order to switch branches. This approach does that in some sense by using the tangent of a perturbation.
- For Hopf and other bifurcations the null vector ϕ_k at the singular point is of a different class than the other null vectors. For example, $\phi_0, \dots, \phi_{k-1}$ may be in \mathbb{R}^n , while ϕ_k is in $\mathbb{R}^n \times S^1$. All this means is that the other null vectors must be promoted to the larger space, since the tangent space $\tilde{\Phi}$ at the perturbed point is in the larger space.

3. Examples.

3.1. Cusp. Our first example is a complexified cusp [8].

$$(x + iy) * ((x + iy)^2 + \lambda) = \mu.$$

This is $n = 4$, $k = 2$, and we can easily find an initial solution $x_0 = y_0 = 0$ at $\mu_0 = 0$, $\lambda_0 = 1$. Figure 3.1 shows $x + y$ as a function of (λ, μ) . The single initial point, with the branch switching algorithm described in the preceding section were sufficient to compute the four regular connected components. Note that the blue components ($y = 0$) are the cusp catastrophe.

3.2. (2,4) cell interaction model. Our second example is a model of the (2,4) cell mode interaction in Taylor-Couette flow ([12] pages 106–110). It is based on an analysis of a two eigenvalue bifurcation by Andreichikov [2], with coefficients computed by Bolstad [4]. The computation of the coefficients is as described in [13]. At radius ratio $\eta = 0.615$ and a 12×48 grid the bifurcation point was found to be at Reynolds number $R = 78.53836$, aspect ratio $\lambda = 2.881799$. The model is

$$x(x^2 + a_1 y^2 - f_1 + b_1 y) = 0$$

$$y(a_2 x^2 + y^2 - f_2) + b_2 x^2 = 0$$

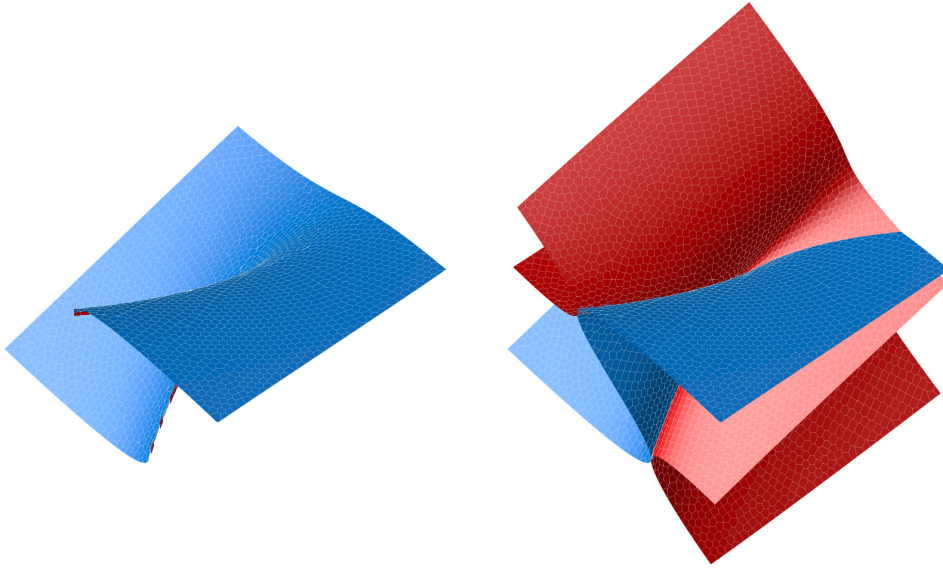


FIG. 3.1. A computation of solutions of $u(u^2 - \lambda) = \mu$. The projection used for rendering is $(\mu, \lambda, x + y)$. (left) Γ_0 , the regular component connected to the initial point. (right) all components ($y \neq 0$ is red, $y = 0$ is blue).

where

$$\begin{aligned}
 a_1 &= 3.67 \\
 b_1 &= -0.0975 - 0.00392\Delta R + 0.0543\Delta\lambda \\
 f_1 &= 0.00117\Delta R - 0.0137\Delta\lambda - 0.00000427\Delta R^2 - 0.000407\Delta R\Delta\lambda + 0.00106\Delta\lambda^2 \\
 a_2 &= 1.19 \\
 b_2 &= 0.0331 + 0.000476\Delta R - 0.00546\Delta\lambda \\
 f_2 &= 0.000681\Delta R + 0.00955\Delta\lambda - 0.000002605^2 - 0.000216\Delta R\Delta\lambda - 0.004925\Delta\lambda^2.
 \end{aligned}$$

The solution manifold consists of three pieces with different symmetries:

- $x = 0, y = 0$ – The trivial solutions.
- $x = 0, y \neq 0$ – The 4-cell solutions. $y^2 - f_2(\Delta R, \Delta\lambda) = 0$.
- $x \neq 0, y \neq 0$ – The mixed 2-cell/4-cell solutions.

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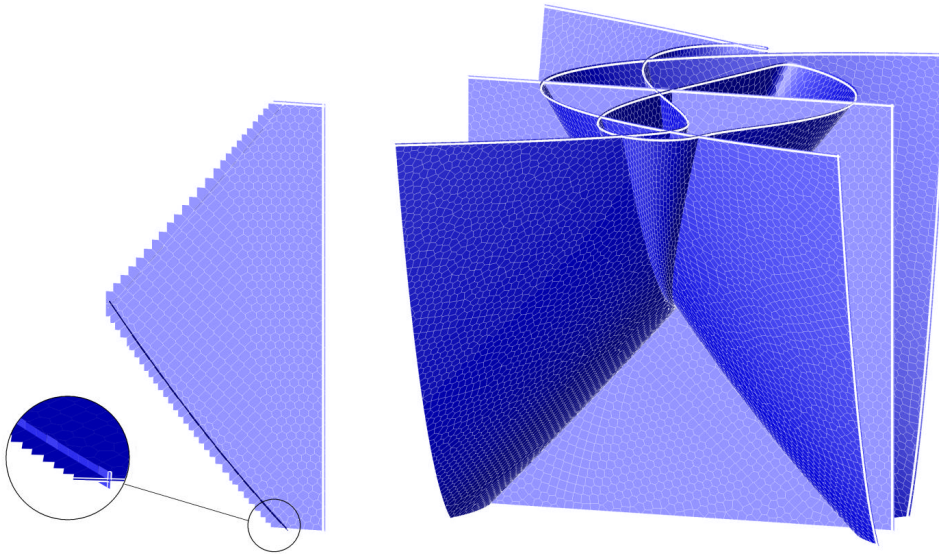


FIG. 3.2. A computation of solutions of a Model for the $(2,4)$ mode interaction in Taylor-Couette flow. The projection used for rendering is $(\Delta R, \Delta \lambda, x + y)$. (left) Γ_0 , the regular component connected to the initial point. The inset shows tiles created using $\{\sigma_0, \dots, \sigma_{k-2}, \phi_k\}$ (right) all components.

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