

**Computation of Homoclinic  
Bifurcations of PDEs Using a Multiple  
Shooting Newton-Picard Method**

*Zuochang Zheng*

*Dirk Roose*

*Report TW 288, December 1998*



**Katholieke Universiteit Leuven**  
Department of Computer Science  
Celestijnenlaan 200A – B-3001 Heverlee (Belgium)

# Computation of Homoclinic Bifurcations of PDEs Using a Multiple Shooting Newton-Picard Method

*Zuochang Zheng*  
*Dirk Roose*

*Report TW 288, December 1998*

Department of Computer Science, K.U.Leuven

## **Abstract**

Periodic solutions of large scale ODE systems, resulting from the space discretization of a PDE system, can be computed efficiently using a shooting method, in which the nonlinear system is solved by a Newton-Picard iteration. For strongly unstable periodic solutions, a multiple shooting approach is necessary. This is for example the case for a periodic solution, approaching a homoclinic orbit, for which some of the Floquet multipliers tend to infinity. In this paper, we describe how a multiple shooting Newton-Picard method can be used to compute homoclinic bifurcations by solving a periodic boundary value problem. This is illustrated with results for a homoclinic bifurcation in the Kuramoto-Sivashinsky Equation.

**Keywords :** PDE, Homoclinic Bifurcation, Newton-Picard.

**AMS(MOS) Classification :** Primary : 65N35, Secondary : 35B32.

# Computation of Homoclinic Bifurcations of PDEs Using a Multiple Shooting Newton-Picard Method

Zuochang Zheng and Dirk Roose  
Katholieke Universiteit Leuven  
Celestijnenlaan 200 A  
B-3001 Heverlee-Leuven, Belgium

Email: Dirk.Roose@cs.kuleuven.ac.be

## Abstract

Periodic solutions of large scale ODE systems, resulting from the space discretization of a PDE system, can be computed efficiently using a shooting method, in which the nonlinear system is solved by a Newton-Picard iteration. For strongly unstable periodic solutions, a multiple shooting approach is necessary. This is for example the case for a periodic solution, approaching a homoclinic orbit, for which some of the Floquet multipliers tend to infinity. In this paper, we describe how a multiple shooting Newton-Picard method can be used to compute homoclinic bifurcations by solving a periodic boundary value problem. This is illustrated with results for a homoclinic bifurcation in the Kuramoto-Sivashinsky Equation.

**Key Words:** PDE, Homoclinic Bifurcation, Newton-Picard Method  
**AMS(MOS) subject classifications** 65N12,35B10,35B32

## 1 Introduction

We consider a large scale one-parameter ODE system

$$\dot{x}(t) = F(x(t), \lambda), \quad x \in R^N, \lambda \in R, N \gg 1 \quad (1)$$

arising from the space discretization of a PDE system. We assume that the ODE system (1) retains the homoclinic bifurcations of the PDE system. Let  $x^h(t)$  be a homoclinic orbit of (1) at  $\lambda = \lambda^h$ , that is,  $x^h(t)$  is a solution of the boundary value problem (BVP) of (1) with boundary conditions  $x^h(\pm\infty) = p(\lambda^h)$ , where  $p(\lambda)$  is a fixed point of (1). To compute the homoclinic bifurcation efficiently, we consider the homoclinic orbit as a periodic solution with infinite period and approximate it by a periodic solution with finite period. Specifically, for a given period  $T > 0$ , we

solve the following periodic boundary value problem

$$\begin{cases} \dot{x}(t) = F(x(t), \lambda), & x \in R^N, \lambda \in R, N \gg 1 \\ x(0) = x(T) \\ g(x, \lambda) = 0 \end{cases} \quad (2)$$

for  $(x^p(t; T), \lambda^p)$  as an approximation to  $(x^h(t), \lambda^h)$ . Here  $g(x, \lambda) = 0$  is a phase condition to fix the time origin. Usually the given period  $T$  must not be taken very large to obtain a reasonable approximation. Indeed, according to the theoretical analysis of Beyn [5], [6], the eigenvalues of the local linearization vector field of the fixed point  $p(\lambda^h)$  determine how large the period  $T$  should be taken to achieve a reasonable accuracy.

For  $N \gg 1$ , the periodic boundary value problem (2) may be prohibitively expensive to solve. Newton-Picard methods based on single or multiple shooting are efficient methods for computing periodic solutions of a PDE system if the periodic solutions have low dimensional dynamics, i.e, if most of the Floquet multipliers are very small in modulus. Many PDEs of practical importance have low dimensional dynamics near steady state solutions. This implies that most of the eigenvalues of a fixed point  $p(\lambda)$  of (1) have a large negative real part. Then numerically most of the nontrivial Floquet multipliers of the periodic solution  $x^p(t; T)$  go to zero and the other nontrivial Floquet multipliers tend to infinity as  $x^p(t; T)$  approaches the homoclinic orbit, see e.g.[7]. Hence a Newton-Picard method can be used to solve the periodic boundary value problem (2), but a multiple shooting method is needed due to numerical instability caused by the large Floquet multipliers.

There are some other advantages to use Newton-Picard methods for computing homoclinic bifurcations. The Newton-Picard method can be used in a continuation process to trace a branch of periodic solutions. During the continuation process, the information about the dominant Floquet multipliers is computed and monitored. Thus an initial guess for the solution of periodic boundary value problem (2) can be obtained cheaply. The information about the Floquet multipliers is further useful to detect the homoclinic bifurcation according to the behaviour of the Floquet multipliers when the periodic solution approaches the homoclinic orbit [7].

In this paper, we describe how a multiple shooting Newton-Picard method can be used efficiently to compute homoclinic bifurcations of a PDE system. In the next section, we formulate a multiple shooting Newton-Picard method for a periodic boundary value problem with a given period  $T$ . Then in section 3, we describe how to use the multiple shooting Newton-Picard method efficiently to compute the homoclinic bifurcations of the PDE system by solving the periodic boundary value problem (2). The method is illustrated in the last section by computing a homoclinic bifurcation of the Kuramoto-Sivashinsky Equation.

## 2 Newton-Picard Method for Periodic Solutions

We now start with describing the multiple shooting method. Let  $\Delta = \{t_i\}_{i=0}^{i=m}$  be a partition of the time interval  $[0, T]$  such that

$$0 = t_0 < t_1 < \cdots < t_m = T \quad (3)$$

We will call  $t_i$ ,  $i = 0, \dots, m$ , the mesh points. Let  $\Delta t_i = t_{i+1} - t_i$  and  $\phi(t, x(0), \lambda)$  be the solution of the ODE system (1) at  $t$  with initial value  $x(0)$ . We determine the values  $x(t_i) = s_i \in R^N$ ,  $i = 0, \dots, m$  with  $s_0 = s_m$ , and  $\lambda$  by solving the algebraic equations

$$\begin{cases} \phi(\Delta t_{i-1}, s_{i-1}, \lambda) = s_i, & i = 1, \dots, m \\ g(s_0, s_1, \dots, s_{m-1}, \lambda) = 0 \end{cases} \quad (4)$$

Usually (4) is solved by Newton iteration. For a given approximation  $s_i^0$ ,  $i = 0, \dots, m-1$ , and  $\lambda^0$ , a full Newton step consists of the following iteration

$$\begin{cases} s_i^1 = s_i^0 + \Delta s_i, & i = 0, \dots, m-1 \\ \lambda^1 = \lambda^0 + \Delta \lambda \end{cases} \quad (5)$$

where  $\Delta s_i$ ,  $\Delta \lambda$  are obtained by solving the linear system

$$\begin{bmatrix} G_1 & -I & & & & b_1 \\ & G_2 & -I & & & b_2 \\ & & \ddots & \ddots & & \vdots \\ & & & G_{m-1} & -I & b_{m-1} \\ -I & & & & G_m & b_m \\ g_1 & g_2 & \cdots & g_m & g_\lambda & \end{bmatrix} \begin{bmatrix} \Delta s_0 \\ \Delta s_1 \\ \vdots \\ \Delta s_{m-2} \\ \Delta s_{m-1} \\ \Delta \lambda \end{bmatrix} = - \begin{bmatrix} r_1 \\ r_2 \\ \vdots \\ r_{m-1} \\ r_m \\ g \end{bmatrix} \quad (6)$$

with

$$\begin{cases} G_i = \frac{\partial \phi(t, x(0), \lambda)}{\partial x(0)} \Big|_{(\Delta t_{i-1}, s_{i-1}^0, \lambda^0)} \\ b_i = \frac{\partial \phi(t, x(0), \lambda)}{\partial \lambda} \Big|_{(\Delta t_{i-1}, s_{i-1}^0, \lambda^0)} \\ r_i = \phi(t, x(0), \lambda) \Big|_{(\Delta t_{i-1}, s_{i-1}^0, \lambda^0)} - s_i^0 \\ g_i = \frac{\partial g}{\partial s_{i-1}} \Big|_{(s_0^0, s_1^0, \dots, s_{m-1}^0, \lambda^0)} \\ g_\lambda = \frac{\partial g}{\partial \lambda} \Big|_{(s_0^0, s_1^0, \dots, s_{m-1}^0, \lambda^0)} \end{cases} \quad (7)$$

When all  $s_i^0$  lie on the periodic solution, for  $i = 0, \dots, m-1$ , the product matrix  $M_i = G_i G_{i-1} \cdots G_1 G_m \cdots G_{i+1}$  is Monodromy matrix. All Monodromy matrices have the same eigenvalues which are called Floquet multipliers, but they may have different eigenvectors.

Normally, the linearized equation (6) is first built explicitly and then solved. The construction of the coefficient matrix requires  $N$  time integrations from 0 to  $T$  of an  $N$  dimensional system. For  $N \gg 1$ , this is prohibitively expensive. The main computational cost lies in the construction and solution of the linearized system (6). If the periodic solution has low dimensional dynamics, i.e., the Floquet multipliers satisfy the relation

$$|\nu_1| \geq \cdots \geq |\nu_p| > \rho > |\nu_{p+1}| \geq \cdots \geq |\nu_N| \quad (8)$$

where the positive integer  $p \ll N$  and  $0 < \rho < 1$ , then a Newton-Picard method can be used to reduce the computational cost without explicitly building the coefficient matrix of the linearized system (6). In the following, we present the main ideas of the method. More detailed information about Newton-Picard methods for computing periodic solutions of a PDE can be found in [1].

A Newton-Picard method computes a spectral decomposition of the Monodromy matrix  $M_i$  corresponding to the invariant subspace  $U_i$  of the first  $p$  dominant Floquet multipliers  $\nu_1, \dots, \nu_p$ , and its orthogonal complement  $U_i^\perp$ ,  $i = 0, \dots, m-1$ . The linearized equation (6) is then projected onto the product spaces  $U_0 \otimes U_1 \otimes \cdots \otimes U_{m-1}$  and  $U_0^\perp \otimes U_1^\perp \otimes \cdots \otimes U_{m-1}^\perp$ , and a separate numerical method is applied to solve the two resulting subsystems. For the large subsystem corresponding to the product space  $U_0^\perp \otimes U_1^\perp \otimes \cdots \otimes U_{m-1}^\perp$ , a cheap method such as Picard iteration can be used since the spectral radius of its coefficient matrix is smaller than 1. To formulate the decomposition, we denote an orthonormal basis for  $U_i$  and  $U_i^\perp$  by  $V_{p,i}$  and  $V_{q,i}$  respectively. The Newton correction  $\Delta s_i \in R^N$  has a unique decomposition  $\Delta s_i = V_{p,i} \Delta \bar{p}_i + V_{q,i} \Delta \bar{q}_i$  with  $\Delta \bar{p}_i \in R^p$  and  $\Delta \bar{q}_i \in R^{N-p}$ . Projecting the equations in (6) which are related to  $G_i$  onto  $U_i$  and  $U_i^\perp$  respectively, we obtain

$$\begin{bmatrix} F_1 & -I & & & & \bar{b}_1 \\ & F_2 & -I & & & \bar{b}_2 \\ & & \ddots & \ddots & & \vdots \\ & & & F_{m-1} & -I & \bar{b}_{m-1} \\ -I & & & & F_m & \bar{b}_m \\ \bar{g}_1 & \bar{g}_2 & \cdots & & \bar{g}_m & g_\lambda \end{bmatrix} \begin{bmatrix} \Delta \bar{q}_0 \\ \Delta \bar{p}_0 \\ \vdots \\ \Delta \bar{q}_{m-1} \\ \Delta \bar{p}_{m-1} \\ \Delta \lambda \end{bmatrix} = - \begin{bmatrix} r_{q,1} \\ r_{p,1} \\ \vdots \\ r_{q,m-1} \\ r_{p,m-1} \\ r_{q,m} \\ r_{p,m} \\ g \end{bmatrix} \quad (9)$$

where

$$\left\{ \begin{array}{l} F_i = \begin{bmatrix} F_{i,1} & F_{i,2} \\ F_{i,3} & F_{i,4} \end{bmatrix} = \begin{bmatrix} V_{q,i}^T G_i V_{q,i-1} & V_{q,i}^T G_i V_{p,i-1} \\ V_{p,i}^T G_i V_{q,i-1} & V_{p,i}^T G_i V_{p,i-1} \end{bmatrix} \\ \bar{b}_i = \begin{bmatrix} b_{q,i} \\ b_{p,i} \end{bmatrix} = \begin{bmatrix} V_{q,i}^T b_i \\ V_{p,i}^T b_i \end{bmatrix}, \bar{r}_i = \begin{bmatrix} r_{q,i} \\ r_{p,i} \end{bmatrix} = \begin{bmatrix} V_{q,i}^T r_i \\ V_{p,i}^T r_i \end{bmatrix} \\ \bar{g}_i = [g_{q,i}, g_{p,i}] = [g_i V_{q,i-1}, g_i V_{p,i-1}] \\ i = 1, \dots, m \end{array} \right. \quad (10)$$

It is straightforward to verify that  $G_i V_{p,i-1} \in U_i$  with  $U_m = U_0$ . We have  $F_{i,2} = V_{q,i}^T (G_i V_{p,i-1}) = 0_{q,p}$ , for  $i = 1, \dots, m$ . Thus in equation (9), the components  $\Delta \bar{q}_i$  are decoupled from the components  $\Delta \bar{p}_i$ . After reordering both equation (9) and the unknowns, moving the terms related to  $\Delta \lambda$  to the right hand side, we extract the large subsystem corresponding to  $U_0^\perp \otimes U_1^\perp \otimes \dots \otimes U_{m-1}^\perp$ , i.e, the so-called Q-system

$$\begin{bmatrix} F_{1,1} & -I_q & & & \\ & F_{2,1} & -I_q & & \\ & & \ddots & \ddots & \\ & & & F_{m-1,1} & -I_q \\ -I_q & & & & F_{m,1} \end{bmatrix} \begin{bmatrix} \Delta \bar{q}_0 \\ \Delta \bar{q}_1 \\ \vdots \\ \Delta \bar{q}_{m-1} \end{bmatrix} = - \begin{bmatrix} r_{q,1} + b_{q,1} \Delta \lambda \\ r_{q,1} + b_{q,2} \Delta \lambda \\ \vdots \\ r_{q,m-1} + b_{q,m-1} \Delta \lambda \\ r_{q,m} + b_{q,m} \Delta \lambda \end{bmatrix} \quad (11)$$

where  $I_q$  is a  $(N-p) \times (N-p)$  identity matrix. The solution of system (11) is computed from the superposition

$$\Delta \bar{q}_i = \Delta \bar{q}_{r,i} + \Delta \lambda \Delta \bar{q}_{b,i}, \quad i = 0, \dots, m-1 \quad (12)$$

where  $\Delta \bar{q}_{r,i}$  and  $\Delta \bar{q}_{b,i}$  are obtained respectively by solving the Q-system (11) with the two right hand sides

$$\left\{ \begin{array}{l} -(r_{q,1}, r_{q,2}, \dots, r_{q,m})^T, \\ -(b_{q,1}, b_{q,2}, \dots, b_{q,m})^T. \end{array} \right. \quad (13)$$

Substituting (12) in the remainder of (9), moving the known terms to the right hand side and combining the terms related to  $\Delta \lambda$ , we obtain the subsystem corresponding to  $U_0 \otimes U_1 \otimes \dots \otimes U_{m-1}$ , i.e, the so-called P-system for  $\Delta \bar{p}_i$  and  $\Delta \lambda$

$$\begin{bmatrix} F_{1,4} & -I_p & & & \tilde{b}_{p,1} \\ & F_{2,4} & -I_p & & \tilde{b}_{p,2} \\ & & \ddots & \ddots & \vdots \\ & & & F_{m-1,4} & -I_p & \tilde{b}_{p,m-1} \\ -I_p & & & & F_{m,4} & \tilde{b}_{p,m} \\ g_{p,1} & g_{p,2} & \dots & g_{p,m} & \tilde{g}_\lambda \end{bmatrix} \begin{bmatrix} \Delta \bar{p}_0 \\ \Delta \bar{p}_1 \\ \vdots \\ \Delta \bar{p}_{m-1} \\ \Delta \lambda \end{bmatrix} = - \begin{bmatrix} \tilde{r}_{p,1} \\ \tilde{r}_{p,2} \\ \vdots \\ \tilde{r}_{p,m-1} \\ \tilde{r}_{p,m} \\ \tilde{g} \end{bmatrix} \quad (14)$$

with

$$\begin{cases} \tilde{b}_{p,i} = b_{p,i} + F_{i,3} \Delta \bar{q}_{b,i} \\ \tilde{r}_{p,i} = r_{p,i} + F_{i,3} \Delta \bar{q}_{r,i} \\ \tilde{g}_\lambda = g_\lambda + \sum_{i=1}^m g_{q,i} \Delta \bar{q}_{b,i} \\ \tilde{g} = g + \sum_{i=1}^m g_{q,i} \Delta \bar{q}_{r,i} \\ i = 1, \dots, m \end{cases} \quad (15)$$

We have now replaced the full Newton iteration by the following three subtasks

1. compute a basis for  $U_0 \otimes U_1 \otimes \dots \otimes U_{m-1}$ ;
2. solve the high dimensional Q-system (11) in a cheap way;
3. solve the low dimensional P-system (14).

To reduce the computational cost, we should achieve all of these subtasks using only a limited number of time integrations of the linearized equations.

First, we note that  $\bar{V}_{p,i} = G_i V_{p,i-1}$  forms a basis for  $U_i$ . Hence to compute the basis vectors  $V_{p,i}$  ( $i = 0, \dots, m-1$ ), we first compute  $V_{p,0}$ , then for  $i = 1, \dots, m$ , the product  $G_i V_{p,i-1}$  and its QR decomposition  $V_{p,i} S_i$ , where  $S_i$  is a  $1 \times 1$  or  $2 \times 2$  block upper triangular matrix of order  $p$ .  $V_{p,0}$  and  $V_{p,m}$  may be two different orthonormal bases for  $U_0$ . To make the description simple, we shall take  $V_{p,0}$  to be the basis for  $U_0$ . A subspace iteration method with projection is applied to compute  $V_{p,0}$ . For the  $k$ -th subspace iteration, the projection matrix  $U = (V_{p,0}^k)^T M_0 V_{p,0}^k = S_{m+1} S_m \dots S_1$  with  $S_{m+1} = (V_{p,0}^k)^T V_{p,m}^k$ . Since the difference between the largest and smallest eigenvalue of the projection matrix  $U$  is very large, it is difficult to compute all basis vectors in  $V_{p,0}$  accurately. Instead of computing the basis vector  $V_{p,0}$  directly, we further perform the periodic Schur decomposition of  $(S_1, S_2, \dots, S_{m+1})$

$$\begin{cases} Y_i R_i = S_i Y_{i-1}, & i = 1, \dots, m \\ Y_0 R_{m+1} = S_{m+1} Y_m \end{cases} \quad (16)$$

with  $Y_i$  a  $p \times p$  orthonormal matrix and  $R_i$  a  $1 \times 1$  or  $2 \times 2$  block upper triangular matrix of order  $p$ . We have the Schur decomposition of the projection matrix  $U Y_0 = Y_0 (R_{m+1} R_m \dots R_1)$  and the updated basis vector  $V_{p,i}^k Y_i$ ,  $i = 0, \dots, m-1$  for the  $k$ -th subspace iteration. To compute the matrix-vector product term  $G_i V_{p,i-1}^k$  without explicitly constructing  $G_i$ , we compute it in full vector form, i.e, in  $R^N$  by integrating the homogeneous linearization equation

$$\dot{y}(t) = F_x(x^0(t), \lambda^0) y(t) \quad (17)$$

from  $t_i$  to  $t_{i+1}$  with initial values  $V_{p,i-1}^k \in R^N$ . Here  $(x^0(t), \lambda^0)$  is an initial solution of (2) with  $x^0(t_i) = s_i^0$ . Note that the convergence factor for a simple eigenvalue  $\nu_i$

is  $|\nu_{p+1}/\nu_i|$ , where  $\nu_{p+1}$  is the next most dominant eigenvalue of  $M_i$ . Usually the integer  $p$  is unknown. Thus during the computation of the basis vectors, we will use  $p_e$  additional vectors to accelerate the convergence of the first  $p$  basis vectors and to make sure that no eigenvalues larger than  $\rho$  are missed.

Second, we need to solve the high dimensional Q-system (11) in a cheap way. To this end, let symbol  $*$   $\in \{r, b\}$ , we condense the Q-system by the forward recursion

$$\begin{aligned} & \text{for } i = 1, \dots, m, \text{ do} \\ & \quad \begin{cases} \Delta \bar{q}_{*,i} = F_{i,1} \Delta \bar{q}_{*,i-1} + *_{q,i} \\ \Delta \bar{q}_{*,m} = \Delta \bar{q}_{*,0} \end{cases} \\ & \text{endfor} \end{aligned} \quad (18)$$

and obtain the condensed system

$$\bar{q}_{*,0} = (F_{m,1} \cdots F_{2,1} F_{1,1}) \Delta \bar{q}_{*,0} + b_{q,*} \quad (19)$$

with

$$b_{q,*} = \sum_{i=1}^m F_{m,1} \cdots F_{i+1,1} *_{q,i} \quad (20)$$

The spectral radius  $r_\sigma(F_{m,1} \cdots F_{2,1} F_{1,1})$  of the condensed system (19) is

$$|\nu_{p+1}| < \rho < 1. \quad (21)$$

Thus the condensed Q-system (19) can be solved by a Picard iteration. Then the other q-components  $\Delta \bar{q}_{*,i}$ ,  $i \neq 0$ , can be obtained by the forward recursion (18). In fact, both the Picard iteration and the other q-components can be computed by the forward recursion (18). To avoid computing  $V_{q,i}$ , the forward recursion (18) must be performed in a full vector form

$$\begin{aligned} & \text{for } i = 1, \dots, m, \text{ compute} \\ & \quad \begin{cases} \Delta q_{*,i} = Q_i G_i \Delta q_{*,i-1} + Q_i *_{q,i} \\ \Delta q_{*,m} = \Delta q_{*,0} \end{cases} \\ & \text{endfor} \end{aligned} \quad (22)$$

Here  $\Delta q_{*,i} = V_{q,i} \Delta \bar{q}_{*,i}$  and  $Q_i = I - V_{p,i} V_{p,i}^T$ . The term  $G_i \Delta q_{*,i-1}$  can also be computed by integrating the homogeneous linearization equation (17) from  $t_{i-1}$  to  $t_i$  with the initial value  $\Delta q_{*,i-1}$ . Similarly,  $b_i$  can be computed by integrating the nonhomogeneous linearization equation

$$\dot{y}(t) = F_x(x^0(t), \lambda^0) y(t) + F_\lambda(x^0(t), \lambda^0) \quad (23)$$

from  $t_{i-1}$  to  $t_i$  with a zero initial value.

After the computation of the basis and the solution of the Q-system, no more time integrations are needed to build the P-system. In fact, it is easy to verify that

after the subspace iterations have converged, with the updated basis vectors, the diagonal blocks of the P-system  $F_{i,4} = R_i$  for  $i = 1, \dots, m-1$  and  $F_{m,4} = R_{m+1}R_m$ . The other terms are built during the solution of the Q-system. Similarly to the Q-system, the P-system can be condensed by the backward recursion

$$\begin{aligned}
 & \text{for } i = m, \dots, 1, \text{ do} \\
 & \quad \begin{cases} \Delta \bar{p}_{i-1} = F_{i,4}^{-1} \Delta \bar{p}_i - F_{i,4}^{-1} (\tilde{b}_{p,i} \Delta \lambda + \tilde{r}_{p,i}) \\ \sum_{i=1}^m g_{p,i} \Delta \bar{p}_{i-1} + \tilde{g}_\lambda \Delta \lambda + \tilde{g} = 0 \\ \Delta \bar{p}_m = \Delta \bar{p}_0 \end{cases} \\
 & \text{endfor}
 \end{aligned} \tag{24}$$

to obtain the condensed P-system

$$\begin{bmatrix} I_p - A_p & c_\lambda \\ o_p & d_\lambda \end{bmatrix} \begin{bmatrix} \Delta \bar{p}_0 \\ \Delta \lambda \end{bmatrix} = - \begin{bmatrix} r_p \\ r_\lambda \end{bmatrix} \tag{25}$$

where

$$\begin{cases} A_p = F_{1,4}^{-1} \cdots F_{m-1,4}^{-1} F_{m,4}^{-1} \\ c_\lambda = \sum_{i=1}^m F_{1,4}^{-1} \cdots F_{i,4}^{-1} \tilde{b}_{p,i} \\ r_p = \sum_{i=1}^m F_{1,4}^{-1} \cdots F_{i,4}^{-1} \tilde{r}_{p,i} \\ o_p = \sum_{i=1}^m g_{p,i} F_{i,4}^{-1} \cdots F_{m,4}^{-1} \\ d_\lambda = \tilde{g}_\lambda - \sum_{i=1}^m g_{p,i} (\sum_{j=i}^m F_{i,4}^{-1} \cdots F_{j,4}^{-1} \tilde{b}_{p,j}) \\ r_\lambda = \tilde{g} - \sum_{i=1}^m g_{p,i} (\sum_{j=i}^m F_{i,4}^{-1} \cdots F_{j,4}^{-1} \tilde{b}_{r,j}) \end{cases} \tag{26}$$

The condensed P-system (25) for  $\Delta \bar{p}_0$  and  $\Delta \lambda$  is small and can be solved using a direct method. Then the other  $\Delta \bar{p}_i$  can be computed from the backward recursion (24). The quantities in (26) can be computed easily by solving at each mesh point a few small linear equations with coefficient matrix  $F_{i,4}$ , which is a  $1 \times 1$  or  $2 \times 2$  block diagonal matrix of order  $p$ .

For a large scale periodic boundary value problem ( $N \gg 1$ ) and a small  $p$ , the overall cost is determined by the number of Newton-Picard iterations necessary for convergence and the cost per Newton-Picard iteration. It is shown in [1] that the overall convergence rate is dominated by the convergence rate (21) of the Picard iterations. During a Newton-Picard iteration,  $p + p_e$  time integrations of the linearization equation (17) are needed to compute the basis vectors. Further 3 time integrations of the linearization equations (17) and (23) are needed. Usually the initial solutions are only known at the mesh points. Thus one time integration of ODE (1) are needed per Picard and Subspace iteration. The total number of time integrations per Newton-Picard iteration is

$$N_{IVP} = (p + p_e + 1) \times N_S + 4 \times N_P \tag{27}$$

Here  $N_S$  and  $N_P$  denote the numbers of subspace iterations and Picard iterations, respectively.  $N_{IVP}$  is independent of the dimension  $N$  of the ODE system (1) and much smaller than  $N$  if  $p + p_e$ ,  $N_S$  and  $N_P$  are small integers. Thus we can conclude that if the periodic solution has low dimensional dynamics, the multiple shooting Newton-Picard method is a cheap method for solving the large scale periodic boundary value problem (2).

### 3 A Newton-Picard Method for Computing Homoclinic Bifurcations

Many PDEs of practical importance has low dimensional dynamics, i.e, their long term dynamical behaviour occurs in a low dimensional manifold of the state space. This is in particular true for steady state solutions. For the ODE (1), we can assume that the fixed point  $p(\lambda^h)$  has low dimensional dynamics, i.e, most of its eigenvalues have a large negative real part and only a few have a positive real part. In [7], we show that the periodic solution  $x^p(t; T)$  also has low dimensional dynamics. Its Floquet multipliers satisfy

$$|\nu_1| \geq \cdots \geq |\nu_{p-1}| > \nu_p = 1 > |\nu_{p+1}| \geq \cdots \geq |\nu_N| \quad (28)$$

The integer  $p$ , the number of dominant Floquet multipliers, is determined by the relative size of the real part of the eigenvalues of the fixed point  $p(\lambda^h)$ . Usually  $p$  is 2 or 3 and can easily be determined. Numerically the nontrivial Floquet multipliers  $\nu_i$  ( $i \neq p$ ) expand to infinity or contract to zero at an exponential rate as the period  $T$  tends to infinity. For a given suitably large period  $T > 0$ , we have  $|\nu_{p-1}| \gg 1$  and  $|\nu_{p+1}| \ll 1$ . Thus the multiple shooting Newton-Picard method described in the last section can be used efficiently to solve the large scale periodic boundary value problem (2). Moreover, we now explain the particular properties of the Floquet multipliers can be used to make the multiple shooting Newton-Picard method for solving (2) cheaper, compared to the computation of general periodic solutions. Indeed, the total number of time integrations per Newton-Picard iteration  $N_{IVP}$  is smaller than that in the computation of general periodic solutions.

For a general periodic boundary value problem,  $p$ , the number of the basis vectors used in a Newton-Picard iteration is unknown and to speed up the convergence of subspace iterations,  $p_e$  extra basis vectors are used. In our case, the integer  $p$  is given. Since  $\frac{|\nu_{i+1}|}{|\nu_i|}$  tends to zero at an exponential rate as the period goes to infinity, the Floquet multipliers are well separated. Thus the subspace iteration converges fast and no extra basis vectors are needed. In our computations,  $N_S$  is taken to be less than 3. In fact, if the number of the basis vectors is taken to be  $\bar{p} > p$ , then  $|\nu_1|$ , which tends to infinity at an exponential rate, is very large

compared to  $|\nu_{\bar{p}}|$  which goes to zero at an exponential rate. The computed smaller Floquet multipliers are very inaccurate. This badly affects the subspace iteration. We should take the number of the basis vectors exactly to be  $p$ . Moreover, since the difference between  $\nu_{i+1}$  and  $\nu_i$  grows at an exponential rate, a lock scheme in the subspace iterations will be quite efficient to further speed up the convergence.

The asymptotic convergence factor of the Picard iterations is  $|\nu_{p+1}|$  which goes to zero at an exponential rate as the period  $T$  tends to infinity. Thus the Picard iteration converges fast. In our computations, no more than 3 Picard iterations are performed. Since the overall convergence of the Newton-Picard iteration is dominated by the convergence rate of the Picard iterations, this implies that the Newton-Picard iteration also converges quite fast.

The discussion above seems to indicate that a larger period  $T$  makes all the iteration procedures converge faster. However, as  $T$  becomes quite large, the first  $p - 1$  dominant Floquet multipliers will be too large. The numerical stability of time integrations will become worse and the condition number of the P-system also increases. This may damage the computation of Newton-Picard iterations. Thus it is important to choose a reasonably large period. An adaptive period selection strategy should be developed. To this end, the information from the subspace iterations and building of the P-system is useful. The information is also useful to develop an adaptive mesh selection strategy. In conclusion, with a suitably chosen period  $T$ , for solving the periodic boundary value problem (2) by the multiple shooting Newton-Picard method, the total number of time integrations is

$$N_{IVP} = (p + 1) \times N_S + 4 \times N_P \quad (29)$$

where the integers  $p$ ,  $N_S$  and  $N_P$  are quite small. For large  $N$ , we have that  $N_{IVP} \ll N$ , i.e, the multiple shooting Newton-Picard method is efficient to compute the homoclinic bifurcations of the PDE system.

## 4 Numerical Examples

To illustrate our conclusion numerically, we have implemented the multiple shooting Newton-Picard method to solve the periodic boundary value problem (2) in Matlab. A Matlab code of the periodic Schur decomposition written by K.Lust [1] is used in the computation of the basis for  $U_0 \otimes U_1 \otimes \cdots \otimes U_{m-1}$ . We computed a homoclinic bifurcation of Kuramoto-Sivashinsky equation (K-S equation)

$$\frac{\partial u}{\partial t} + 4 \frac{\partial^4 u}{\partial x^4} + \alpha \left( \frac{\partial^2 u}{\partial x^2} + u \frac{\partial u}{\partial x} \right) = 0 \quad (30)$$

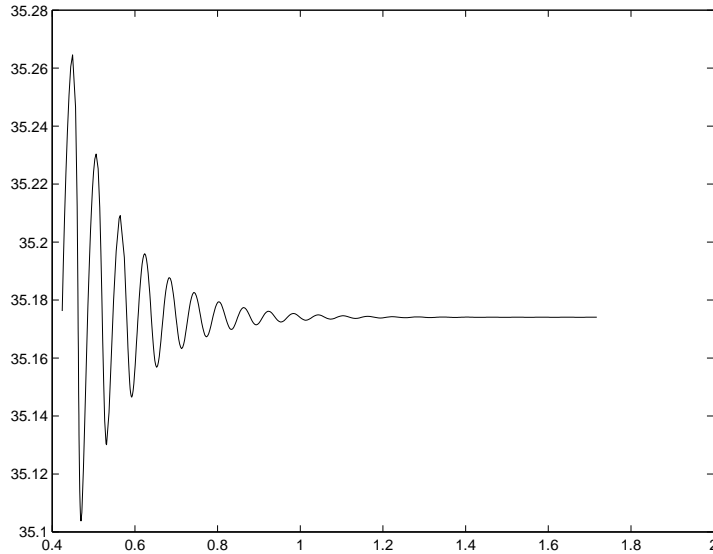


Figure 1: Bifurcation diagram of a periodic solution branch for the K-S equation. The periodic solution branch terminates at a homoclinic orbit.

Following Jolly et al [8], we discretize the K-S equation using a  $N$ -mode spatial spectral approximation

$$u(x, t) = \sum_{k=1}^N b_k(t) \sin(kx) \quad (31)$$

and obtain the ODE system

$$\frac{db_k(t)}{dt} = (-4k^4 + \alpha k^2)b_k - \alpha \beta_k, \quad 1 \leq k \leq N \quad (32)$$

where  $\beta_k = \frac{1}{2} \sum_{j=1}^N j b_j [b_{k+j} + \text{sign}(k-j)b_{|k-j|}]$  with  $b_j = 0$  if  $j < 0$  or  $j > N$ . Generally speaking, when  $N \geq 8$ , the ODE system (32) has the same long term dynamics as the K-S equation itself for the parameter interval  $\alpha \in [0, 70]$ . In particular, there are two branches of steady state solutions, each of which has a Hopf point at  $\alpha = 34.299$ . The numerical computations presented in [8] show that the periodic solutions bifurcating from the two Hopf points terminate at a homoclinic orbit when  $\alpha = \alpha^* \simeq 35.174066$ . We focus on one of the two periodic solution branches. The fixed point where the homoclinic orbits emanates has a pair of complex eigenvalues. The homoclinic orbit has a spiraling structure. We have computed the periodic solution for the 8-mode discretization of the K-S equation ( $N = 8$ ) with  $\alpha = 35.20$  and period  $T = 0.572362$  using AUTO97 and used it as a starting point for a continuation process with the period  $T$  as the continuation parameter. We used a classical embedding method. The periodic solution branch

<i>Eigenvalues of fixed point</i>		<i>Real</i>
<i>Real part</i>	<i>Imaginary part</i>	<i>Floquet multipliers</i>
7.8152504E+00	-1.0452187E+02	9.9997384E-01
7.8152504E+00	1.0452187E+02	-3.6455148E-13
-3.5554418E+01	0.0000000E+00	-8.5525090E-20
-4.3258700E+02	0.0000000E+00	6.8230858E-18
-1.6085723E+03	0.0000000E+00	1.4981425E-19
-3.9081603E+03	0.0000000E+00	7.1584459E-18
-7.8728384E+03	0.0000000E+00	5.1133315E-19
-1.4111208E+04	0.0000000E+00	4.4722867E+11

Table 1: Kuramoto-Sivashinsky equation: The eigenvalues of the fixed point and the Floquet multipliers of the periodic solutions with  $\alpha = 3.5174067E + 01$ .

undergoes a lot of turning-point bifurcations as shown in Figure 1. We selected 8 points from the initial solution as multiple shooting mesh points. During the continuation process, the time mesh has been updated every continuation step. Following [1], we use a partition of the time interval with  $t_0 = 0$  and  $t_{i+1} = t_i + (\sigma_{i+1} - \sigma_i)T, i = 0, \dots, m - 1$ , and where

$$0 = \sigma_0 < \sigma_1 < \dots < \sigma_m = 1 \quad (33)$$

are fixed. Thus we update the time mesh by perturbing each mesh point with a perturbation proportional to the ratio of the periods corresponding to two successive continuation steps.

In our computations, we used  $\sigma_0 = 0, \sigma_1 = 0.101, \sigma_2 = 0.1888, \sigma_3 = 0.3290, \sigma_4 = 0.4026, \sigma_5 = 0.5886, \sigma_6 = 0.8838, \sigma_7 = 1$ . With a continuation step  $\Delta T = 1.0E - 03$ , the periodic solution branch can be traced until  $T = 0.580362$  and  $\alpha = 35.173846 \simeq \alpha^*$ . This periodic solution is close to the homoclinic orbit. In a Newton-Picard iteration, 2 subspace iterations and 2 Picard iterations are needed. Since one of the Floquet multipliers tends to infinity, we take  $p = 2$ . Table 1 contains the eigenvalues of the fixed point and the Floquet multipliers of the periodic solution with  $\alpha = 3.5174067E + 01$ . In fact, when  $p > 2$ , the computation of the basis vectors fails. According to (29), the total number of time integrations per Newton-Picard iteration is 14. Note that for a full Newton implementation of a multiple shooting method only requires  $N + 1 = 9$  time integrations per full Newton step. However, the number of time integrations per Newton-Picard step does not depend on  $N$ , the dimension of the ODE system, but only depends on the distribution (8) of the Floquet multipliers. For large scale ODE systems, the multiple shooting Newton-Picard is cheaper than the classical multiple shooting method. We have also computed an approximation to the homoclinic bifurcation for  $N = 16$ . Taking an initial solution with  $\alpha = 3.519629E + 01$  and period  $T = 6.237399E - 01$ , we trace the periodic solution branch until  $\alpha = 3.517428E + 01$  and  $T = 7.237399E - 01$ . Since the largest multipliers are larger than in the 8-mode

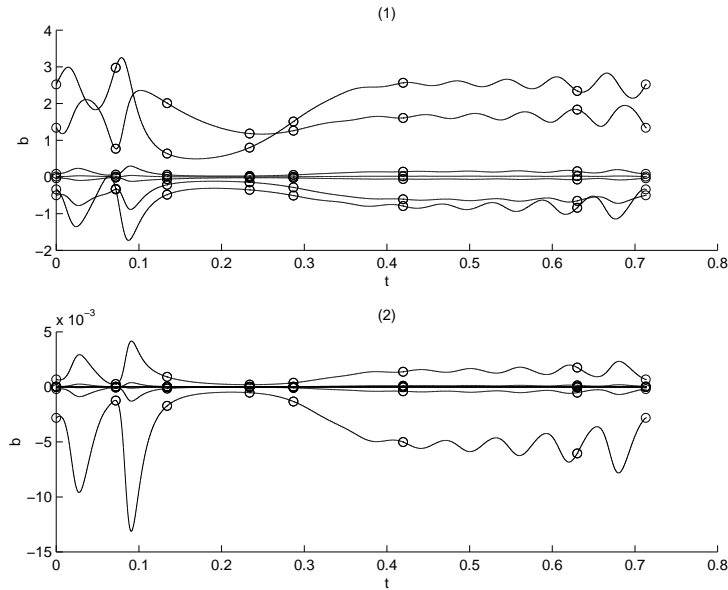


Figure 2: The periodic solution for the K-S equation with period= 7.237399E-01 and parameter=3.517428E+01. It is computed using a multiple shooting Newton-Picard method. 1) the computed solution curves of  $b_j$ ,  $j = 1, \dots, 7$ ; 2) the computed solution curves of  $b_j$ ,  $j = 8, \dots, 16$ .

case, the periodic solutions are more difficult to solve numerically. The distribution of the Floquet multipliers is qualitatively the same as in the 8-mode case. Thus in this case, we can still take  $p = 2$ . Only 2 subspace and Picard iterations are needed per Newton-Picard iteration during our computations. Thus the total number of time integrations is again 14. The computed solution curve is shown in Figure 2.

In conclusion, our numerical computations verify that the number of time integrations per Newton-Picard iteration is independent of  $N$  and for large scale problems, the multiple shooting Newton-Picard method is an efficient method for computing homoclinic bifurcations of a PDE system, even if the periodic solutions are quite close to the homoclinic orbit.

## References

- [1] Kurt Lust, Numerical bifurcation analysis of periodic solutions of partial differential equations, Ph.D. Thesis, Katholieke Universiteit Leuven, 1997.
- [2] K. Lust, D. Roose, A. Spence, and A.R. Champneys, An adaptive Newton-Picard algorithm with subspace iteration for computing periodic solutions, SIAM J. Sci. Comput., 19(4), 1998, pp. 1188-1209.

- [3] K. Lust and D. Roose, Computation and bifurcation analysis of periodic solutions of large-scale systems, IMA Preprint 1536, February, 1998.
- [4] D. Roose, K. Lust, A. Champneys, and A. Spence, A Newton-Picard shooting method for computing periodic solutions of large-scale dynamical systems, *Chaos, Solitons & Fractals*, 5(10), 1995, pp. 1913-1925.
- [5] W.J. Beyn, Numerical Computation of Connecting Orbits in Dynamical Systems, *IMA J. of Numerical Analysis* (9), 1990, pp. 379-405.
- [6] W.J. Beyn, Global Bifurcations and Their Numerical Computation, in *Continuation and Bifurcations: Numerical Techniques and Applications*, edited by D. Roose et al, 1990, pp. 169-182.
- [7] Z.C. Zheng and D. Roose, On the Behaviour of the Floquet Multipliers of Periodic Solutions Near a Homoclinic Orbit, Report TW 287, Department of Computer Science, Katholieke Universiteit Leuven, 1998.
- [8] M.S. Jolly, I.G. Kevorkidis and E.S. Titi, Approximate Inertial Manifolds for the Kuramoto-Sivashinsky Equations: Analysis and Computations *Physica D* (44), 1990, pp. 38-60.