WAVETRAIN

Software for Studying Periodic Travelling Wave Solutions of Partial Differential Equations

Jonathan A. Sherratt

Dept of Mathematics and Maxwell Institute for Mathematical Sciences, Heriot-Watt University, Edinburgh EH14 4AS, UK.

If you publish research done using this software, please cite
J.A. Sherratt: Numerical continuation methods for studying periodic travelling wave (wavetrain) solutions of partial differential equations. Submitted.

If your research includes results on wave stability, please also cite
J.D.M. Rademacher, B. Sandstede, A. Scheel: Computing absolute and essential spectra using continuation. Physica D 229, 166-183 (2007).
and
J.A. Sherratt: Numerical continuation of boundaries in parameter space between stable and unstable periodic travelling wave (wavetrain) solutions of partial differential equations. Submitted.

This user guide is for version wavetrain0.1

Copyright © 2011 by Heriot-Watt University, Edinburgh, UK. All rights reserved worldwide. Printing of parts or the whole of this document for the purposes of research or private study, or criticism or review, are permitted. No part of this document or the related files may be distributed by any means (electronic, photocopying, recording, or otherwise) without the prior written permission of either Heriot-Watt University or the author. All requests for such permission should be sent by e-mail to `j.a.sherratt@hw.ac.uk`; please include the word wavetrain (upper or lower case) in the subject heading.

Limit of Liability and Disclaimer of Warranty: The information provided in this document is provided "as is". Heriot-Watt University and the author make no representation or warranties with respect to the accuracy or completeness of the contents of this document and specifically disclaim any implied warranties of merchantability or fitness for any particular purpose. Under no circumstances will Heriot-Watt University or the author be liable for any loss of use, interruption of business or any direct, indirect, special, incidental, and/or consequential damages of any kind (including loss of profits) even if Heriot-Watt University or the author have been advised of the possibility of such damages. Neither Heriot-Watt University nor the author warrant that this document will be error-free.

Contents

How to Use this User Guide

This user guide is rather long. However, new users should be reassured that only a relatively small proportion of it is needed in order to begin using WAVETRAIN. Part 1 of the user guide contains some introductory comments, followed by details of the installation procedure and of some post-installation tests. Part 2 is an introductory description of the package, via two examples, that explain how to use WAVETRAIN. Part 3 is concerned with more advanced features, and is intended for users who already have some familiarity with the package. Part 4 is a reference section, containing lists of commands and details of output data files.

In order to facilitate the printing of individual parts of this user guide, page numbering begins with the title page being page 1. This means that page selections in the print window give user guide pages with the same numbers.

Restrictions on Distribution

The WAVETRAIN software and this user guide are both freely available. However, please note that the formal statements on page 2 and in §1.4 specify that neither the user guide nor the software (in whole or in part) can be distributed in either electronic or printed (or any other) form. In particular, you cannot post this user guide or the information it contains, or part or all of the WAVETRAIN software, on any electronic bulletin board, web site, FTP site, newsgroup, or similar forum. The only places from which either the WAVETRAIN software or this document should be available are the WAVETRAIN web site `www.ma.hw.ac.uk/wavetrain` and the authors' web site `www.ma.hw.ac.uk/~jas`. Please respect this restriction: one of the reasons for it is to ensure that new users always download the most up-to-date version of the software and user guide.

Part 1

Introduction to WAVETRAIN and Installation

1.1 Aims and Scope

WAVETRAIN is a software package for investigating periodic travelling wave solutions of partial differential equations. Typically such equations will contain a number of parameters. WAVETRAIN requires that one of these be selected; this parameter will be termed the control parameter throughout this user guide. Focussing on periodic travelling waves introduces an additional parameter, the wave speed. The basic task performed by WAVETRAIN is the calculation of the region of the control parameter–wave speed plane in which periodic travelling waves exist, and additionally where they are stable.

WAVETRAIN is suitable for systems of equations with only single time derivatives, which can be coupled with equations involving space derivatives only. Mixed space and time derivatives are not allowed. Specifically, WAVETRAIN can be used to study systems of $N \geq 1$ equations whose form is either

$$\partial u_i/\partial t = F_i\left(\underline{u}, \partial\underline{u}/\partial x, \partial^2\underline{u}/\partial x^2, \partial^3\underline{u}/\partial x^3, \ldots\right), \quad 1 \leq i \leq N \tag{1.1a}$$

or

$$\partial u_i/\partial t = F_i\left(\underline{u}, \partial\underline{u}/\partial x, \partial^2\underline{u}/\partial x^2, \partial^3\underline{u}/\partial x^3, \ldots\right), \quad 1 \leq i < M \tag{1.1b}$$

$$0 = F_i\left(\underline{u}, \partial\underline{u}/\partial x, \partial^2\underline{u}/\partial x^2, \partial^3\underline{u}/\partial x^3, \ldots\right), \quad M \leq i \leq N \tag{1.1c}$$

where $2 \leq M \leq N$. There is no upper limit on N or on the order of spatial derivatives on the right hand side of the equations.[†]

The three main underlying principles of WAVETRAIN are that it should

(i) be easy to use, even for users with limited mathematical background;

(ii) produce publication-quality graphical output that can be fine-tuned by the user if required;

[†]In fact, there is an upper limit on N: some of the temporary files created during WAVETRAIN runs are formatted under the assumption that $N < 2 \times 10^6$. This is not expected to be a limitation in any practical situation.

(iii) provide detailed output data files that are accessible to the user if required, and that have an easily comprehensible format.

Once the user has acquired some familiarity with WAVETRAIN, application to a new problem should require a relatively small amount of user time. However, users should be aware that some of the computations may involve significant computer time; such runs can be performed in the background.

1.2 System Requirements

WAVETRAIN requires a unix or linux operating system. Users with Windows or Macintosh operating systems can use WAVETRAIN via a virtual machine, for which there is freely available software; see for example `www.virtualbox.org/wiki`. After downloading a virtual machine, the user will have to download a linux operating system, such as the freely available Ubuntu linux (`www.ubuntu.com/download/ubuntu/download`). One of the systems on which WAVETRAIN has been tested is an AMD64 PC running `Oracle VM VirtualBox` with the `ubuntu-11.04-desktop-i386` operating system. Once a virtual machine and linux operating system have been downloaded, one simply opens the virtual machine and follows the installation procedure. For example, opening the `Oracle VM VirtualBox` gives the options `New`, `Settings`, `Start` and `Discard`. Selecting "`New`" opens a Virtual machine wizard window which guides the user through the setup of a new Operating system; the VirtualBox user guide (`www.virtualbox.org/wiki/Documentation`) provides additional help if required.

WAVETRAIN also requires a Fortran77 compiler that is compatible with some extensions to the Fortran77 standard. Details of how to check whether your system has a suitable compiler are given in §1.7; if it does not, a number of suitable compilers are freely available. For example, WAVETRAIN has been tested with the GNU compiler `gfortran-4.0`, downloaded from the website `packages.ubuntu.com/dapper/gfortran`.

Graphical output in WAVETRAIN can be performed using either `gnuplot` or `sm`. The plotting commands are the same for both plotting packages. The `gnuplot` package is supplied automatically on almost all unix and linux operating systems, but if if needs to be installed, it is freely available from `www.gnuplot.info`. The `sm` package is commercial but inexpensive, and can be obtained from `www.supermongo.net`. WAVETRAIN graphics were originally developed using `sm`, and users with `sm` are recommended to use this rather than `gnuplot` because it processes data files more quickly. However, it is anticipated that most users will use `gnuplot`. The plots generated by the two plotters are completely equivalent. The figures in this user guide were generated using `sm`.

To check whether `gnuplot` is installed on your system, simply type `gnuplot` at the system prompt. Either an error message will appear indicating that `gnuplot` is not installed, or `gnuplot` will start. In the latter case, type

```
show version long
```

at the `gnuplot>` prompt. This will give details of the version of `gnuplot` and various details of the compilation. WAVETRAIN requires version 4.2 or higher of `gnuplot`, and

requires that it has been compiled with the following options enabled: macro expansion, string variables, and data strings. These options will be indicated by "`+MACROS`", "`+STRINGVARS`" and "`+DATASTRINGS`" being listed amongst the compile options. If one of these criteria are not met, then it will be necessary to reinstall or recompile `gnuplot` before it can be used as the plotter for WAVETRAIN. By default, WAVETRAIN uses `wxt` as the `gnuplot` plotting terminal. To confirm that this is available on your system, type

```
set terminal wxt 0 enhanced font "Sans,10"
```

at the `gnuplot>` prompt. If an error message appears, it will be necessary to edit the file `defaults.input` in order to change the terminal setting; see §3.4.1.1 for details.

To exit `gnuplot`, type `quit` at the `gnuplot>` prompt.

1.3 Authorship

WAVETRAIN was written by Jonathan Sherratt. It includes (with permission) software from several other packages:

AUTO97, developed by Eusebius Doedel (currently Concordia University, formerly California Institute of Technology) and coworkers (`indy.cs.concordia.ca/auto`; Doedel, 1981; Doedel *et al*, 1991). AUTO97 is a numerical continuation package that is used extensively by WAVETRAIN. Current AUTO users should note that the relevant parts of the AUTO code are incorporated into WAVETRAIN, which will therefore run independently of existing AUTO settings. Note that previous experience with AUTO is not necessary for using WAVETRAIN. The AUTO97 distribution includes code from the software package EISPACK, a software package for numerical computation of eigenvalues and eigenvectors of matrices, and this code is also distributed as part of WAVETRAIN. EISPACK was developed by Brian Smith and coworkers at Argonne National Laboratory (`www.netlib.org/eispack`; Smith *et al.*, 1976).

LAPACK, a software package for numerical linear algebra developed by researchers at many institutions (`www.netlib.org/lapack`; Anderson *et al.*, 1999). Note that the EISPACK package used by AUTO97 is a forerunner of LAPACK.

BLAS, the Basic Linear Algebra Subprograms, developed by Jack Dongarra (currently University of Tennessee, formally Argonne National Laboratory) and coworkers (`www.netlib.org/blas`; Lawson *et al.*, 1979; Dongarra *et al.*, 1988a,b; Dongarra *et al.*, 1990a,b).

MINPACK, a software package for studying nonlinear systems of algebraic equations, developed by the University of Chicago, as operator of Argonne National Laboratory (`www.netlib.org/minpack`; Moré *et al*, 1984).

1.4 Copyright, Distribution and Disclaimer

Copyright. WAVETRAIN software is intended for free personal private and academic use only and was developed by Jonathan Sherratt at Heriot-Watt University, Edin-

burgh, UK, and is protected by copyright. The copyright owner is Heriot-Watt University, with the exception of the routines from the packages AUTO, BLAS, EISPACK, LAPACK and MINPACK, which are included with permission, which are clearly identified in the source code, and the use of these packages is under the conditions of the original owners which are available at the websites `www.netlib.org/blas/faq.html#2`; `www.netlib.org/lapack/#_licensing`; `www.netlib.org/minpack/disclaimer`.

Persons or organisations wishing to use this WAVETRAIN software for commercial purposes or purposes other than its original intention should contact the owners to request specific written permissions.

Distribution. Distribution of WAVETRAIN software, in part or as a whole, by any means (electronic, printed copy or otherwise), is prohibited without the prior written permission of either Heriot-Watt University or the author Jonathan A. Sherratt. All requests for such permission should be sent by e-mail to `j.a.sherratt@hw.ac.uk`; please include the word wavetrain (upper or lower case) in the subject heading.

Warranty limitations. The product and service are provided "as is". The owner disclaims any and all warranties, including but not limited to, all expressed or implied warranties of merchantability and fitness for a particular purpose. Under no circumstances will the owner be liable to you for any loss of use, interruption of business or any direct, indirect, special, incidental, and/or consequential damages of any kind (including loss of profits) even if the owner has been advised of the possibility of such damages. The owner accepts no legal liability for any of the product and/or service sold, offered for sale, or otherwise made available for public or private consumption in relation to this software. The owner does not warrant that this software will be error-free.

1.5 Acknowledgements

While writing WAVETRAIN, I was supported in part by a Leverhulme Trust Research Fellowship. I would have been incapable of writing WAVETRAIN without my research collaboration with Matthew Smith (Microsoft Research, Cambridge) and Jens Rademacher (CWI, Amsterdam), and I am very grateful to them both for our many discussions. I also thank Philipp Janert and Wasit Limprasert for help with gnuplot, Steve Mowbray for computer advice, Lisa Keyse for secretarial help, and Alan MacDonald and Jennifer Reynolds for testing parts of this user guide. Finally but most importantly, I am deeply grateful to Pam and Dorothy for being so supportive, and for putting up with my many hours in front of the computer screen.

1.6 Feedback

Feedback about WAVETRAIN is strongly encouraged. It is particularly helpful to receive details of any problems experienced in using WAVETRAIN, and any suggestions for improvements that could be included in future releases. Comments about this user guide, including typos, are also very welcome. Positive comments are also permitted! The e-mail address for all feedback is `j.a.sherratt@hw.ac.uk`; please include the word wavetrain (upper or lower case) in the subject heading. Please state in your e-mail which version of

WAVETRAIN you are using; this information is contained in the file `README` in the main WAVETRAIN directory.

1.7 Installation

WAVETRAIN is freely available and can be downloaded from the WAVETRAIN web site `www.ma.hw.ac.uk/wavetrain`. The single file `wavetrain`*n.m*`.tar` should be downloaded; here *n.m* is the version number. This file should be expanded in the usual way, by typing

`tar -xf wavetrain`*n.m*`.tar`

at the system prompt. This will create a directory `wavetrain`*n.m* containing all of the WAVETRAIN files. The directory `wavetrain`*n.m* will be referred to as "the main WAVETRAIN directory" throughout this user guide. The tar file can then be deleted by typing

`rm -f wavetrain`*n.m*`.tar`

although this is not necessary. Now go into the new direcory by typing

`cd wavetrain`*n.m*

and then type

install

which will list the copyright, distribution and disclaimer statement. The user must enter `y` or `Y` at the prompt to confirm that they have read and understood the statement, and that they agree to the conditions.

After completing the installation, it is recommended that the user runs three tests:

Test 1: the search path. WAVETRAIN requires that the current directory (".") is included in the search path. A user already using unix/linux will almost certainly have this setting, but this may not be the case for users who are new to unix/linux. To check this setting, the command

`./pathtest`

should be entered at the system prompt (from within the main WAVETRAIN directory). This will check the search path, and if a change is required, the screen output will contain advice on how to change the search path.

Test 2: the Fortran77 compiler. Once the search path is set appropriately, the user should run a test of the Fortran77 compiler on their system. The default name for the compiler is `f77`, but this can be changed by editting the file `defaults.input` in the directory `input_files`; the compiler name is set on line 15 (see §3.2 for details). To test the compiler, one types the command

`fortrantest`

in the main WAVETRAIN directory. If the resulting screen output is

```
Test completed
```

then the compiler is suitable for WAVETRAIN. If an error message appears, such as "`f77: Command not found`", this indicates that a compiler needs to be installed, or that the name needs to be changed: a number of compilers are freely available. A third possibility is that "`Test completed`" appears, but is preceded by a list of subroutines, such as

```
MAIN:
dotest:
```

which indicates that by default, the compiler operates in a non-silent mode. This type of compiler output will make WAVETRAIN's screen output very difficult to follow, and it should be suppressed. This can be done by editting `defaults.input` in the `input_files` subdirectory (see §3.2) and adding a suitable compiler flag on line 15. The appropriate flag is compiler dependent, but "`-silent`" or "`-fsilent`" are likely possibilities. Having made this change, the `fortrantest` command should be run again to confirm that it has worked.

Test 3: a test run of AUTO97. WAVETRAIN makes extensive use of the numerical continuation software AUTO97 (see §1.3). Having confirmed that the Fortran77 compiler is working appropriately, the user is recommended to test the operation of AUTO97, via the command

```
auto97test
```

(from within the main WAVETRAIN directory). This test will begin by compiling the AUTO97 code. This may not be successful even if `fortrantest` has worked, because AUTO97 uses some extensions to the Fortran77 standard. WAVETRAIN requires that the user's Fortran77 compiler is able to compile the AUTO97 code. If the compilation is successful, the `auto97test` command goes on to perform a test run of AUTO97. If this test run is executed successfully, it will produce a table of numerical values; users who are unfamiliar with AUTO may find this table rather overwhelming, but can be reassured that this test only needs to be performed once. The output should be compared to that shown in Figure 1.1, which is reproduced in the file `auto_test/auto_test/example_output`. The precise numerical values may vary according to computer architecture and Fortran77 compiler; as long as the values produced by the test are approximately the same as in Figure 1.1 and `auto_test/auto_test/example_output`, the test has been successful.

Once these three tests have been completed successfully, the user is ready to begin using WAVETRAIN.

```
 BR    PT   TY  LAB     PAR(1)        L2-NORM          U(1)          U(2)
  1     1   EP    1  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
  1    33   LP    2  1.057390E-01  1.484391E+00  3.110230E-01  1.451441E+00
  1    70   LP    3  8.893185E-02  3.288241E+00  6.889822E-01  3.215250E+00
  1    90   HB    4  1.308998E-01  4.271867E+00  8.950803E-01  4.177042E+00
  1    92   EP    5  1.512417E-01  4.369748E+00  9.155894E-01  4.272750E+00
 BR    PT   TY  LAB     PAR(1)        L2-NORM       MAX U(1)      MAX U(2)
  4    45        6  1.181275E-01  3.609914E+00  9.987721E-01  8.885717E+00
  4    90   EP   7  1.056503E-01  2.219179E+00  9.991661E-01  9.366083E+00
 BR    PT   TY  LAB     PAR(1)        L2-NORM          U(1)          U(2)
  2    27   LP   6  1.353353E-01  2.061424E+00  4.999688E-01  1.999875E+00
  2   100   EP   7  1.092464E-08  2.136635E+01  9.531508E-01  2.134508E+01
 BR    PT   TY  LAB     PAR(1)        L2-NORM          U(1)          U(2)
  4   100   EP   6  8.809076E-05  1.174407E+01  9.146096E-01  1.170841E+01
```

Figure 1.1: The output that should appear on the screen during execution of the command `auto97test`. This is reproduced in the file `auto_test/auto_test/example_output`. Note however that the precise numerical values may vary according to the computer architecture and Fortran77 compiler.

Part 2

How to Use WAVETRAIN

2.1 Getting Started With WAVETRAIN

The main WAVETRAIN directory contains a subdirectory `input_files`. Before starting investigation of a new periodic travelling wave problem, the user must create a subdirectory of `input_files` in which the various input files must be placed. Several such input subdirectories are provided in the installed version of WAVETRAIN, and the input subdirectory `demo` contains the input files for a very simple application of WAVETRAIN, intended as a tutorial case. The equations studied in `demo` are

$$\begin{aligned} \partial u/\partial t &= wu^2 - Bu + \partial^2 u/\partial x^2 \\ \partial w/\partial t &= A - w - wu^2 + \nu \partial w/\partial x. \end{aligned}$$

This is a dimensionless version of a model for vegetation patterns in semi-arid environments, first proposed by Klausmeier (1999). For a more detailed discussion of this problem, and for details of a more systematic study of these equations using WAVETRAIN, see Sherratt (2011a). A description of the various input files is postponed until §2.2, and the remainder of this section consists of an explanation of the use of WAVETRAIN to study the problem in `demo`. New users are encouraged to run the various commands on their own system as they follow the description of this example.

2.1.1 Investigation of Periodic Travelling Wave Existence

The typical starting point for the investigation of periodic travelling waves is a series of partial differential equation simulations in which such waves have been observed. Based on this (or other) information, the user must decide upon a range of values of the control parameter and wave speed over which periodic travelling waves are to be investigated; this information is entered in the input file `parameter_range.input`. For `demo` the range $0.1 < A < 3.4$ and $0.3 < c < 1.1$ has been chosen. Here A has been chosen as the control parameter, and c is the name chosen for the wave speed; these are set in the input file `variables.input`. The first stage in the use of WAVETRAIN is to test the suitability of (some of) the various computational inputs in the file `constants.input` for the particular problem. To do this, one must enter manually a pair of A and c values for which a periodic travelling wave is expected to exist: a good choice is values corresponding

```
This run has been assigned run code 1001
STARTING CALCULATION OF PERIODIC TRAVELLING WAVE SOLUTION

THE AUTO LIBRARIES NEED TO BE CREATED.

THE AUTO SOURCE CODE WILL NOW BE RECOMPILED
NOTE: THIS MAY GENERATE SOME WARNING MESSAGES, DEPENDING
      ON THE FORTRAN COMPILER. THESE ARE NOT EXPECTED TO
      BE A CAUSE FOR CONCERN: THEY WILL NOT BE SHOWN ON
      THE SCREEN, AND WILL NOT BE INCLUDED AS PART
      OF THE ERRORS AND WARNINGS LIST. HOWEVER, THEY
      DO APPEAR IN info.txt IN THE OUTPUT SUBDIRECTORY.

END OF CALCULATION FOR demo WITH pcode=100 rcode=1001

THE OUTCOME WAS:
     PERIODIC TRAVELLING WAVE FOUND, STABILITY NOT REQUESTED
     PERIOD = 0.21580722E+02

THERE WERE NO ERRORS OR WARNINGS DURING THE RUN
```

Figure 2.1: The output that should appear on the screen during the execution of the command `ptw demo 2.0 1.0`. The precise value of the period may vary according to the computer architecture and Fortran77 compiler.

to the observation of a wave in simulations of the partial differential equations. For `demo`, the values $A = 2.0$ and $c = 1.0$ are suitable. One then types

```
ptw demo 2.0 1.0
```

and WAVETRAIN will calculate the corresponding periodic travelling wave. Figure 2.1 shows the screen output that should appear during the run, which should only take a few seconds. The run is allocated a four digit "rcode" (1001-9999) which will be used later to specify the run, for example when plotting. Since this is the first run, the rcode value is 1001, and this is reported in the screen output. One can then calculate the wave for a second pair of control parameter and wave speed values, for example via the command

```
ptw demo 1.5 0.8
```

which is allocated an rcode value of 1002. Often it will be appropriate to run tests for several pairs of values.

The user may wish to plot the periodic travelling waves that have been calculated. To do this, one starts the WAVETRAIN plotter by typing

```
plot demo
```

and one then types

```
@ptw 1001
```

at the plotter prompt to obtain a plot of the first wave that was calculated, and

```
@ptw 1002
```

for the second. The results are illustrated in Figure 2.2. The plotter should then be exitted by typing `@quit` or `@exit`. Note that all plotter commands begin with the "at" character `@`.

Having confirmed that the computational constants are appropriate one can proceed with investigation of the designated section of the A–c parameter plane. The input file `parameter_range.input` also contains the number of points in a grid of (A, c) parameter values over which wave existence will be checked. For `demo`, a 5×3 grid is used. This is extremely coarse, and is chosen to reduce run times for demonstration purposes; typically a 10×10 or 20×20 grid would be used in a real problem. To run over the grid, one types

```
ptw_loop demo
```

and WAVETRAIN will loop through the points in the parameter grid. As will be seen in the screen output, WAVETRAIN allocates a 3 digit "pcode" value to this run (the "p" in pcode stands for "parameter loop"). Apart from rcode values (which are four-digit), all WAVETRAIN code numbers, including pcode values, are three-digit and range from 101 to 999. Since this is the first run to be performed, the pcode value will be 101.

To visualise the results of the run, one starts the WAVETRAIN plotter again by typing

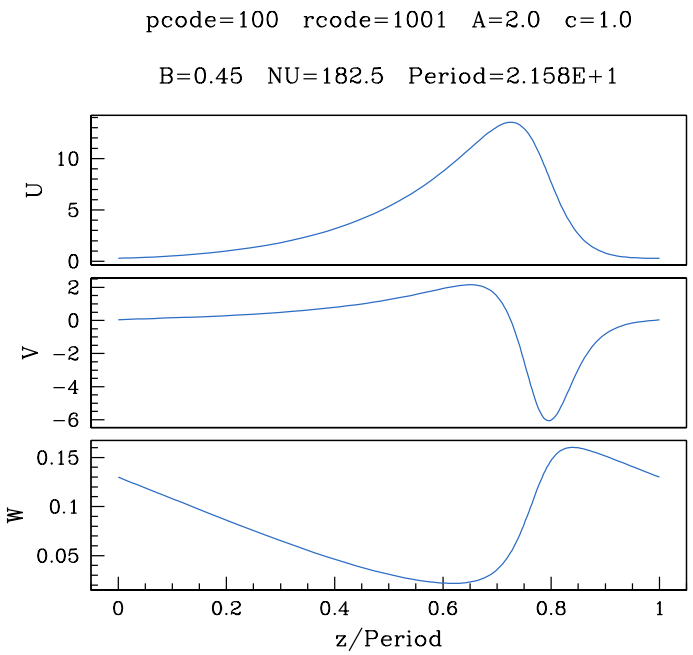
```
plot demo 101
```

(the number 101 is the pcode value) and then types

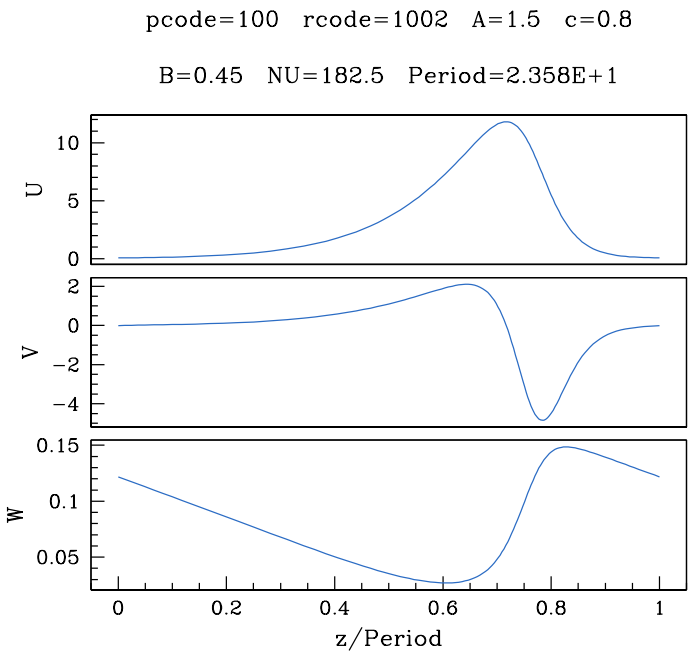
```
@pplane
```

at the plotter prompt. The plotter asks whether or not to use the default setting of labelling the parameter sets by their rcode values. Hitting RETURN (ENTER) to accept this default gives the picture illustrated in Figure 2.3a: the colour of an rcode value indicates the result of the corresponding calculation. Note that a rather small font is used for the rcode values in Figure 2.3a. This default setting is chosen with much finer parameter grids in mind (see for example Figure 3.6 on page 85). However, like most aspects of WAVETRAIN plots, the default font can be changed (see §3.3.1).

A key indicating the meaning of the colours is automatically generated when the plotter is started; it is in the file `pplane_key.eps` in the subdirectory `postscript_files` of the main WAVETRAIN directory. The colours can all be changed if desired (see §3.3.1), but with their default values, the key will be as shown in Figure 2.4. Figure 2.3a shows that there are two different outcomes, depending on the control parameter and wave speed values. For some pairs of values, a periodic travelling wave has been found, while for others it has not. In the latter case, the phrase "no convergence" appears beside the

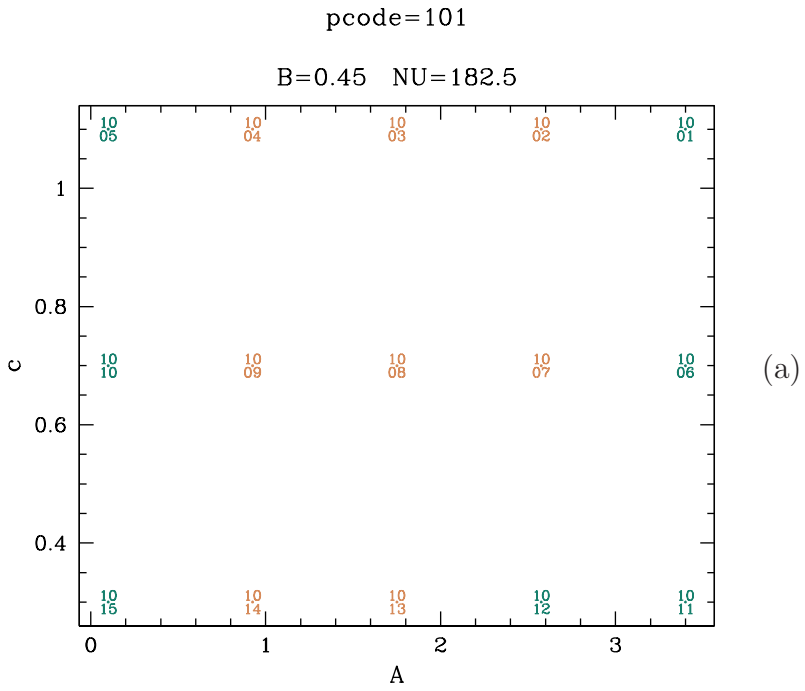


(a)

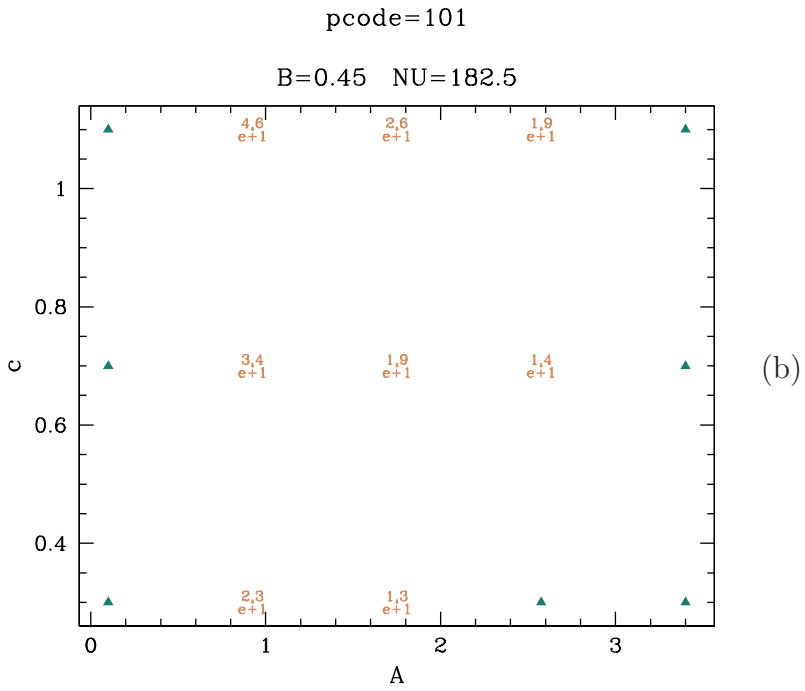


(b)

Figure 2.2: Two periodic travelling wave solutions for the problem `demo`. The run and plot commands used to generate these figures are given in the main text, and are also listed in the Appendix. The first lines of the titles show the pcode and rcode numbers for the run, together with the values of the control parameter A and the wave speed c. The second lines show the periods of the solutions, and also the values of the two parameters B and ν, which appear in the equations but which are not being used as the control parameter; their values are specified in the file `other_parameters.input` (see §2.2.3).



(a)



(b)

Figure 2.3: Results on the existence of periodic travelling wave solutions for the problem `demo`. A key illustrating the meaning of the various colours is shown in Figure 2.4 on page 19. The run and plot commands used to generate these figures are given in the main text, and are also listed in the Appendix.

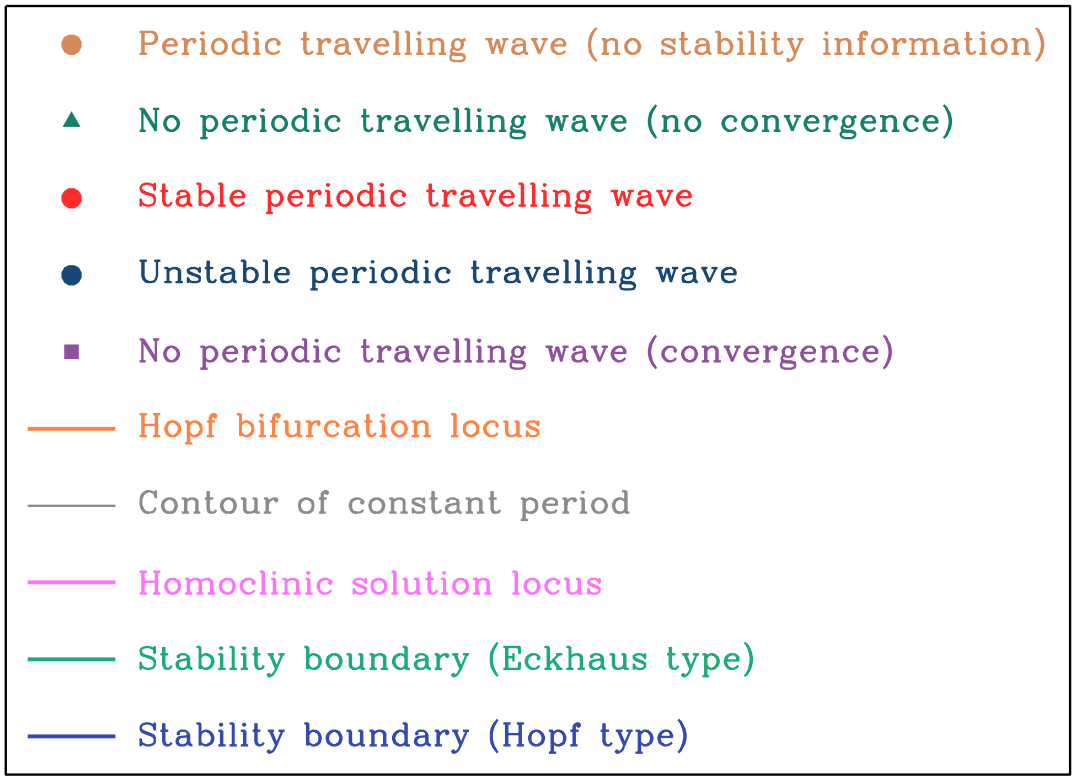


Figure 2.4: The key for the control parameter–wave speed plots, indicating the meaning of the various points and lines. This key is automatically generated when the plotter is started; it is in the file `pplane_key.eps` in the subdirectory `postscript_files` of the main WAVETRAIN directory. The user can specify that only a subset of the lines in this key be included: see §3.3.1 for details on how to change this and other plotter settings. Additionally, if the user wishes to include a key in material for presentation or publication, then they will probably prefer to use a single entry for cases where there is no periodic travelling wave, and correspondingly to have a single entry in the key. This can be achieved by resetting the plotter setting `pplanekeytype` (see §3.3.1).

corresponding colour in the key in Figure 2.4. To search for periodic travelling waves, WAVETRAIN numerically continues periodic travelling waves along the solution branch as the control parameter varies, starting at the Hopf bifurcation point in the travelling wave equations. The phrase "no convergence" indicates that this continuation has ended with a convergence failure because the solution approaches a homoclinic solution (the end of the solution branch) without passing through the required value of the control parameter. There are some situations in which there is no periodic travelling wave but for which continuation finishes without a convergence failure; the WAVETRAIN plotter then uses a different symbol. This issue is discussed in detail in §3.1.8. If the user wishes to include a key in material for presentation or publication, then they will probably prefer not to

include the "no convergence" phrase, and this can be achieved by changing the plotter settings, as explained in §3.3.1.

The form of the periodic travelling wave solutions can again be visualised using the `@ptw` plotter command. Thus

```
@ptw 1007
```

would generate a plot of the wave for $A = 2.575$ and $c = 0.7$, while

```
@ptw 1006
```

would give an error message, since no periodic travelling wave solution was found for this rcode value. Rerunning the `@pplane` plot command but now entering `period` as the label style gives the picture shown in Figure 2.3b; the colours are the same as in the previous picture, but when the wave exists, its period is now displayed. The plotter should now be exitted by typing `@quit` or `@exit`.

At this stage one could proceed with investigation of the stability of the periodic travelling wave solutions, but in this case we will first use WAVETRAIN to obtain more details of the region of the A–c parameter plane in which periodic travelling wave solutions exist. Boundaries of the region can be of two possible types. They can correspond to a Hopf bifurcation in the travelling wave equations, so that the wave amplitude is zero on the boundary. Alternatively, they can correspond to a homoclinic solution, so that the period (wavelength) is infinite. The parameter grid used for `demo` is too coarse to clarify the nature of the left- and right-hand boundaries in Figure 2.3. (The coarse grid is chosen to keep run times small). However with a finer grid, a plot of wave periods such as Figure 2.3b shows that the period increases markedly near the boundary on the left, but not near that on the right. Hence the left-hand boundary corresponds to homoclinic solutions, while the right-hand boundary corresponds to Hopf bifurcation points.

WAVETRAIN can be used to trace these boundaries. From the previous results, it is expected that the Hopf bifurcation locus (right hand boundary) crosses $c = 0.8$ between $A = 2.0$ and $A = 3.5$. Typing

```
hopf_locus demo 101 2.0 0.8 3.5 0.8
```

causes WAVETRAIN to locate this crossing point and then continue the boundary starting from that point. (The number 101 is the pcode value). Similarly, the previous results suggest that the locus of homoclinic solutions (left hand boundary) crosses $c = 0.8$ between $A = 0$ and $A = 1.5$. There is no capability in WAVETRAIN to locate/track true homoclinic solutions but one can approximate the homoclinic (period=∞) locus by the locus of a solution of large finite period. Typing

```
period_contour demo 101 period=3000 1.5 0.8 0.0 0.8
```

causes WAVETRAIN to calculate the contour of period 3000. WAVETRAIN allocates a 3 digit "ccode" number (101-999) to this period contour calculation; since this is the first such calculation to be done, the ccode number is 101. In many cases, one will wish to calculate contours for various different values of the period, and these will be given different code numbers. Thus typing

```
period_contour demo 101 period=80 2.5 0.8 0.5 0.8
```

causes WAVETRAIN to calculate the contour for waves of period 80; the ccode number for this run is 102. The command `list_periods` can be used to list the periods corresponding to the various ccode numbers; thus for instance

```
list_periods demo 101
```

(where 101 is the pcode value) causes WAVETRAIN to report that the period is 3000 for ccode 101 and 80 for ccode 102. An "hcode" number (101-999) is also allocated to a run of `hopf_locus`; this is because in principle there may be more than one Hopf bifurcation locus curve in the chosen part of the A–c plane; however this is not the case for `demo`.

To visualise these new results, one starts the plotter again by typing

```
plot demo 101
```

and then draws the parameter grid results again by typing

```
@pplane
```

at the plotter prompt; for variety, select `symbol` as the plotting type. One can then draw the Hopf bifurcation locus by typing

```
@hopf_locus 101
```

where 101 is the hcode number. If more than one Hopf bifurcation locus has been calculated, the command

```
@hopf_locus all
```

can be used to plot all of them. For the period contours, the separate commands

```
@period_contour 101
```

and

```
@period_contour 102
```

can be used to draw the contour for the two ccode numbers; alternatively the single command

```
@period_contour all
```

will draw them both. In either case, it is appropriate to press RETURN (ENTER) when prompted about the label location, to select default labelling. The plot resulting from these various commands is illustrated in Figure 2.5. The plotter should now be exitted by typing `@quit` or `@exit`.

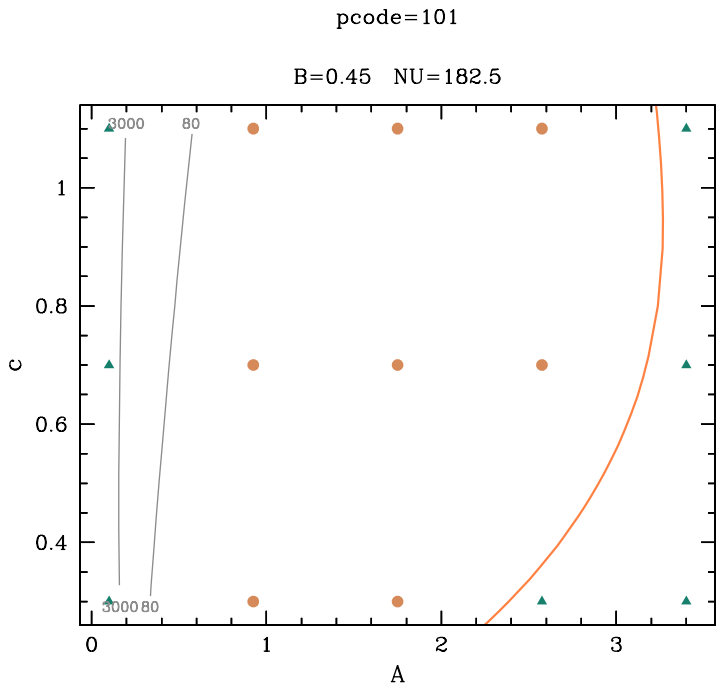


Figure 2.5: The Hopf bifurcation locus and two contours of constant wave period for the problem `demo`, superimposed on a plot showing periodic travelling wave existence in the control parameter–wave speed plane. A key illustrating the meaning of the various colours and symbols is shown in Figure 2.4 on page 19. The run and plot commands used to generate this figure are given in the main text, and are also listed in the Appendix.

2.1.2 Investigation of Periodic Travelling Wave Stability

The calculations and plots described above give a detailed account of the region of the A–c parameter plane in which there are periodic travelling waves, but they give no information about the stability of these waves, which is a fundamental issue in applications (Sherratt & Smith, 2008). WAVETRAIN determines stability by calculating the eigenvalue spectrum via numerical continuation, using the method of Rademacher *et al* (2007). Although a detailed understanding of the method is not needed in order to use WAVETRAIN, a brief introduction will help users with their choice of computational constants. For a periodic travelling wave, the system of equations satisfied by the (complex-valued) eigenfunctions has coefficients that are periodic in the travelling wave coordinate. However, the eigenfunctions themselves need not be periodic; their amplitude must be periodic, but their phase shift γ across one period of the wave is not constrained, and is the central player in the method of Rademacher *et al* (2007). One begins by calculating the eigenvalues for which $\gamma = 0$, i.e. those for which the corresponding eigenfunction is periodic with the same period as the wave. This is done by discretising the eigenfunction equation and then

solving (numerically) the resulting matrix eigenvalue problem. These periodic eigenfunctions and the corresponding eigenvalues can then be used as starting points for numerical continuation in the phase shift γ, which effectively "joins the dots" in the eigenvalue complex plane. Performing this continuation starting from each periodic eigenfunction results in the whole eigenvalue spectrum being traced out. This spectrum will always contain the origin (reflecting the neutral stability of the wave to translations), and the wave is unstable if and only if the spectrum crosses into the right-hand half of the eigenvalue complex plane.

In order to implement this procedure, WAVETRAIN requires two basic computational parameters to be set:

1. The number of periodic eigenfunctions to use as starting points for continuation in γ (`nevalues`). WAVETRAIN uses the eigenvalues with largest real part, considering either eigenvalues with real part ≥ 0, or all eigenvalues, depending on the value of the constant `iposre`.

2. The number of points used in the discretisation of the eigenfunction equations (`nmesh2`).

In principle, the spectrum may undergo a large excursion that crosses the imaginary axis between any pair of consecutive eigenvalues corresponding to periodic eigenfunctions, but in practice it is typical that a relatively small value of `nevalues` (8 or 10 say) is sufficient to capture any crossing of the imaginary axis. For demo, `nevalues` is fixed at 4 to reduce computation time; this would be dangerously low for a real problem.

The choice of `nmesh2` is very important. If it is too low, the discretisation introduces eigenvalues that have no analogue in the actual partial differential equations. However too high a value makes computation times excessive and also introduces significant errors into the matrix eigenvalue calculation (see §3.1.10). The command `eigenvalue_convergence` enables a suitable value of `nmesh2` to be determined. It has a variable (> 3) number of arguments. The first three arguments are the problem name (`demo` in this case) and the values of the control parameter and wave speed being considered; the rest are a list of candidate `nmesh2` values. The command `eigenvalue_convergence` sorts these candidate values into numerical order and calculates the requested number of eigenvalues (according to `nevalues` and `iposre`). Thus

```
eigenvalue_convergence demo 2.4 0.8 5 10 30 100 200
```

calculates the four eigenvalues for `nmesh2` $= 5$, 10, 30, 100 and 200. (Four is the value of `nevalues` set in the input file `constants.input`; see §2.2.1). The run is allocated an "ecode" value (101-999); since this is the first run of `eigenvalue_convergence`, the ecode value is 101. Note that this run takes several minutes on a typical desktop computer.

The `eigenvalue_convergence` command does not display any results itself. Rather the separate command `convergence_table` is used for that purpose. For example, one types

```
convergence_table demo 101 2
```

nmesh	Re of evalue 2	Im of evalue 2	Error bound 2
5	-0.38268891E+00	0.76626544E-01	0.33022440E-12
10	-0.35918911E+00	0.00000000E+00	0.19255672E-11
30	-0.36096484E+00	0.00000000E+00	0.60103036E-11
100	-0.36100219E+00	0.00000000E+00	0.22931134E-10
200	-0.36102336E+00	0.00000000E+00	0.93608241E-10

Figure 2.6: The change in the eigenvalues of the discretised eigenfunction equations as the constant `nmesh2` (defined in `constants.input`) is varied. The run command for this table is `eigenvalue_convergence demo 2.4 0.8 5 10 30 100 200`. Assuming that this is the first run of the `eigenvalue_convergence` command for `demo`, it will be allocated an ecode value of 101. The table shown can then be generated via the command `convergence_table demo 101 2`.

(here 101 is the ecode value) to display a "convergence table", showing how the second out of the four eigenvalues changes as `nmesh2` is varied. Here the eigenvalues are ordered by the size of their real parts. The results are shown in Figure 2.6, but note that the precise numerical values will vary according to computer architecture and the Fortran77 compiler. Alternatively one can use

```
convergence_table demo 101 3 4
```

to display a table using eigenvalues number 3 and 4 (ordered by their real parts), or

```
convergence_table demo 101 all
```

to use all four of the eigenvalues. These commands show that one of the eigenvalues is missing in the (very coarse) discretisation at `nmesh2`=5 but is present at `nmesh2`=10; further increase improves accuracy. The choice `nmesh2`=30 is adequate for the purposes of demo. Note that as well as listing the real and imaginary parts of the eigenvalues, the "convergence table" produced by the "`convergence_table`" command contains an estimated error bound for each eigenvalue displayed. This error bound concerns the numerical errors in the calculation of the matrix eigenvalues. Therefore the displayed eigenvalues are only reliable as matrix eigenvalues if this error bound is significantly smaller in absolute value than both the real and imaginary parts of the calculated eigenvalue.

Having fixed on `nevalues`=4 and `nmesh2`=30, one can test these choices by calculating the eigenvalue spectrum for a typical parameter set. This is done via a command of the form

```
stability demo 2.2 0.8
```

where the second and third arguments are the values of A and c. This run will be given a (four-digit) rcode value, which will be reported in the screen output; since two runs (of the `ptw` command) have been done previously for a specified parameter set, the rcode value will be 1003 in this case. It can be visualised by typing

```
plot demo
```

to start the plotter; no pcode value is needed since the results to be plotted do not come from a parameter plane run. The command

```
@spectrum 1003
```

generates a plot of the eigenvalue spectrum (here 1003 is the rcode value); when prompted about the axes limits, one can just press RETURN (ENTER), since the default settings are appropriate. The resulting plot is illustrated in Figure 2.7; the dots indicate eigenvalues corresponding to periodic eigenfunctions ($\gamma = 0$), and the colours (red–green–blue) indicate the value of γ along the spectrum curves in between. Note that both the colour scheme for the spectrum curves and the marking of eigenvalues corresponding to periodic eigenfunctions are default settings that can be changed (see §3.3.2). As usual, one exits the plotter by typing `@quit` or `@exit`.

Having chosen values of `nevalues` and `nmesh2`, investigation of periodic travelling wave stability using WAVETRAIN is a two stage process. First, one scans the A–c parameter plane looking for regions in which periodic travelling waves are stable/unstable. This is done using the command `stability_loop`, which is directly analogous to `ptw_loop` except that at each parameter point at which a wave exists, its stability is also determined. Thus the command

```
stability_loop demo
```

loops through the points in the parameter plane as specified in `parameter_range.input`. This run will be allocated a new pcode value; since only one previous parameter plane has been determined (using `ptw_loop`), the pcode value is 102. Note that this run of `stability_loop` repeats the computations done previously in the run of `ptw_loop`, since it is necessary to calculate the form of a periodic travelling wave before calculating its spectrum; however this does not increase the computation time significantly, since the majority of the run time is associated with the stability calculation.

To visualise the results, one starts the plotter again by typing

```
plot demo 102
```

(102 is the pcode value) and then types

```
@pplane
```

at the plotter prompt. If the default plot type (`rcode`) is selected, then the resulting plot is illustrated in Figure 2.8; it is very similar to that generated previously by `@pplane` for pcode value 101, but the colours indicating the existence of periodic travelling waves now also show wave stability. It maybe of interest to visualise the eigenvalue spectrum for some of these waves, which can be done using the `@spectrum` plot command. Thus typing

```
@spectrum 1002
```

shows the eigenvalue spectrum for $A = 2.575$ and $c = 1.1$ (illustrated in Figure 2.9a), while

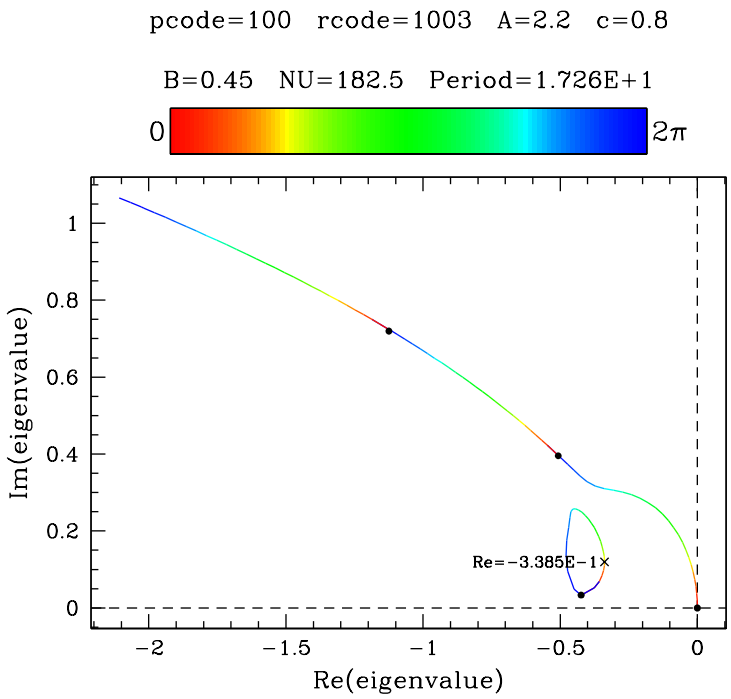


Figure 2.7: The eigenvalue spectrum for one pair of control parameter and wave speed values, for the problem `demo`. The dots indicate eigenvalues corresponding to periodic eigenfunctions, and the colours along the curve indicate the phase difference in the eigenfunction over one period of the periodic travelling wave. The run and plot commands used to generate this figure are given in the main text, and are also listed in the Appendix. The two parameters B and ν, whose values are given in the title, appear in the equations but are not being used as the control parameter. Their values are specified in the file `other_parameters.input` (see §2.2.3). The cross, which is labelled with the corresponding value of the real part of the eigenvalue, indicates the fold in the eigenvalue spectrum with largest real part, other than the origin. The sign of the real part of the eigenvalue at this point is used by WAVETRAIN to classify the wave as either stable or unstable. Note that if plotting is done using `gnuplot` then ticmarks will be absent from the horizontal axis in this plot; this applies if `spectrumcolour` is set to `rainbow` or `greyscale` or `grayscale`, but not if a single colour is used.

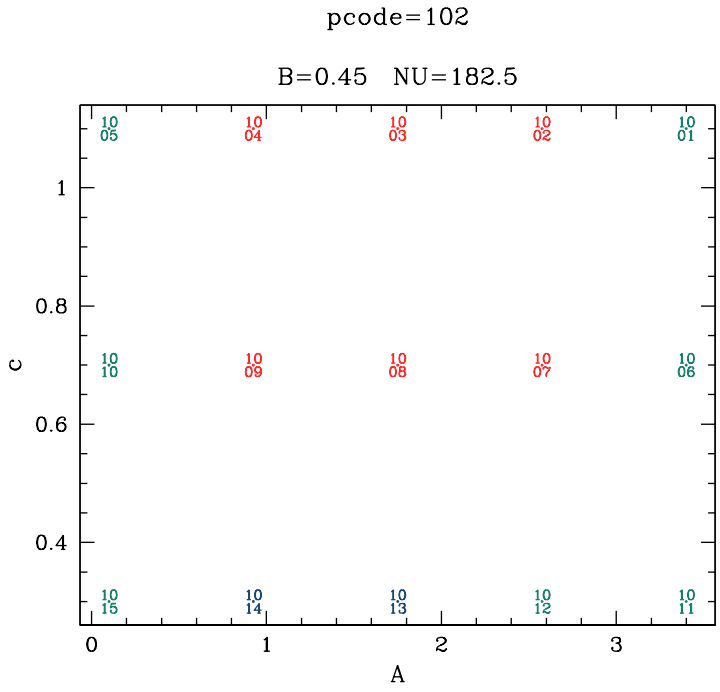


Figure 2.8: Results on the existence and stability of periodic travelling wave solutions for the problem `demo`. A key illustrating the meaning of the various colours is shown in Figure 2.4 on page 19. The run and plot commands used to generate this figure are given in the main text, and are also listed in the Appendix.

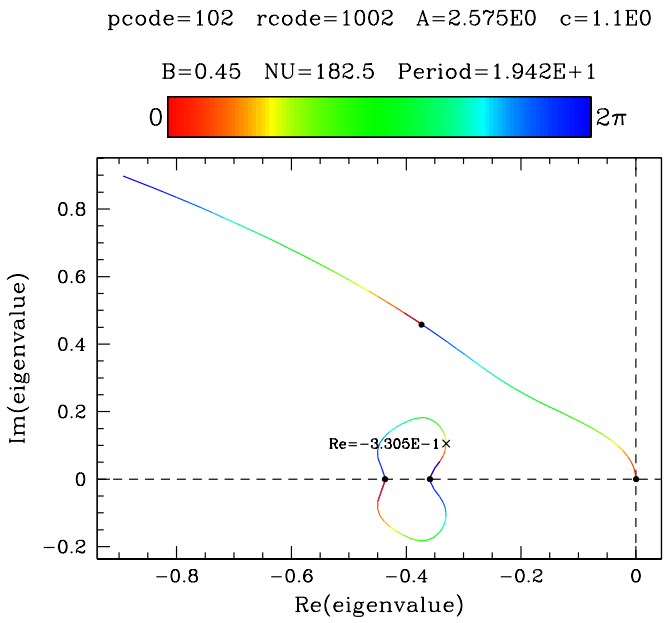
```
@spectrum 1013
```

shows the spectrum for $A = 1.75$ and $c = 0.3$ (illustrated in Figure 2.9b). (In both cases, the default axes limits are appropriate). In the first case, the wave is stable, and the spectrum remains in the left hand half of the complex plane, while in the second case the wave is unstable, and the spectrum crosses the imaginary axis. As usual, one exits the plotter by typing `@quit` or `@exit`.

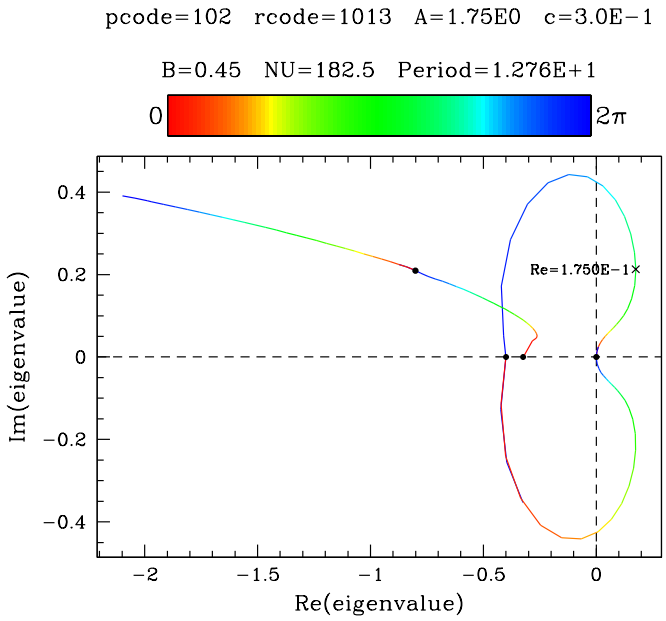
The second stage in determining wave stability is to compute the boundary curve(s) between stable and unstable waves. To do this, WAVETRAIN requires the coordinates of two points in the A–c parameter plane lying either side of the boundary curve: a periodic travelling wave must exist for the first point, but this is not necessary for the second. As for the `hopf_locus` and `period_contour` commands, the two points must either have the same value of A or the same value of c. Based on the results of the scan through the parameter plane, one can therefore enter the command

```
stability_boundary demo 102 1.75 0.3 1.75 0.7
```

to calculate the stability boundary. This run is significantly more time-consuming than the previous runs (5-10 minutes on a typical desktop computer). During the run, various



(a)



(b)

Figure 2.9: The eigenvalue spectrum for two pairs of control parameter and wave speed values, for the problem `demo`. The periodic travelling wave is stable for (a) and unstable for (b). The dots indicate eigenvalues corresponding to periodic eigenfunctions, and the colours along the curve indicate the phase difference in the eigenfunction over one period of the periodic travelling wave. The run and plot commands used to generate these figures are given in the main text, and are also listed in the Appendix. The two parameters B and ν, whose values are given in the titles, appear in the equations but are not being used as the control parameter. Their values are specified in the file `other_parameters.input` (see §2.2.3). Note that if plotting is done using `gnuplot` then ticmarks will be absent from the horizontal axis in these plots; this applies if `spectrumcolour` is set to `rainbow` or `greyscale` or `grayscale`, but not if a single colour is used.

warning messages will appear. The run is given a 3 digit "scode" value (101-999); in this case scode=101 since this is the first stability boundary to be calculated. In general there may be more than one segment of stability boundary in the region of the control parameter–wave speed plane being considered; each can be calculated using different starting coordinates, and they would be allocated different scode values. However, for `demo` there is only one stability boundary curve. Note that the `stability_boundary` command also has optional additional arguments, which are discussed in §3.1.2.

For periodic travelling waves, changes in stability can be of either Eckhaus or Hopf type (see §3.1.11 and Rademacher & Scheel, 2007). The `stability_boundary` command automatically detects which of these occurs. Details of how the `stability_boundary` works are given in §3.1.11, and an example problem with a change in stability of Hopf type is given there; for `demo`, the stability boundary corresponds to a change of Eckhaus type. This is reported in the output information and is available to the plotter, which uses (by default) a different colour for stability boundary curves of the two types. To plot the results one must first generate a parameter plane plot: one restarts the plotter via

```
plot demo 102
```

(102 is the pcode value), and then types

```
@pplane
```

at the plotter prompt, selecting the default plot type. One then superimposes the stability boundary onto this plot via

```
@stability_boundary 101
```

(101 is the scode value); the result is illustrated in Figure 2.10.

The final step in completing the parameter plane plot would be to superimpose the Hopf bifurcation locus and the contours of constant period. These were calculated previously for the same model parameters, but they were computed as part of pcode 101 not pcode 102 and are therefore not currently available to the plotter, which must now be exitted via `@quit` or `@exit`. Of course, one could simply repeat the Hopf bifurcation and period contour calculations for pcode 102, but this is not necessary. Instead one can simply type

```
copy_hopf_loci demo 101 102
```

and

```
copy_period_contours demo 101 102
```

(here 101 and 102 are the two pcode values). These commands copy the previously calculated solutions across. A check is made that the two sets of input files are the same, and then all data files copied; note however that the hcode/ccode numbers may be changed.

All calculations for demo are now completed. To plot the final result, one starts the plotter again via

```
plot demo 102
```

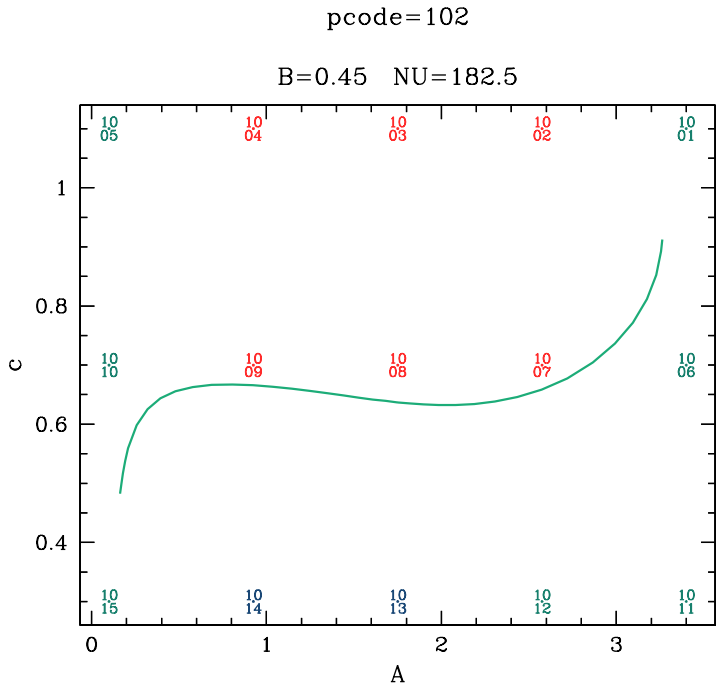


Figure 2.10: The interface between regions of stable and unstable periodic travelling waves, superimposed on results on wave stability, for the problem `demo`. A key illustrating the meaning of the various colours is shown in Figure 2.4 on page 19. The run and plot commands used to generate this figure are given in the main text, and are also listed in the Appendix.

(here 102 is the pcode number) and then enters the relevant series of plot commands:

```
@pplane
```

(to draw the parameter plane, selecting `symbol` as the plot type),

```
@hopf_locus 101
```

(to draw the Hopf bifurcation locus),

```
@period_contour all
```

(to draw the contours of constant period, selecting the default label locations), and

```
@stability_boundary 101
```

(to draw the stability boundary). The resulting plot is illustrated in Figure 2.11. To generate a postscript file of this plot, one types

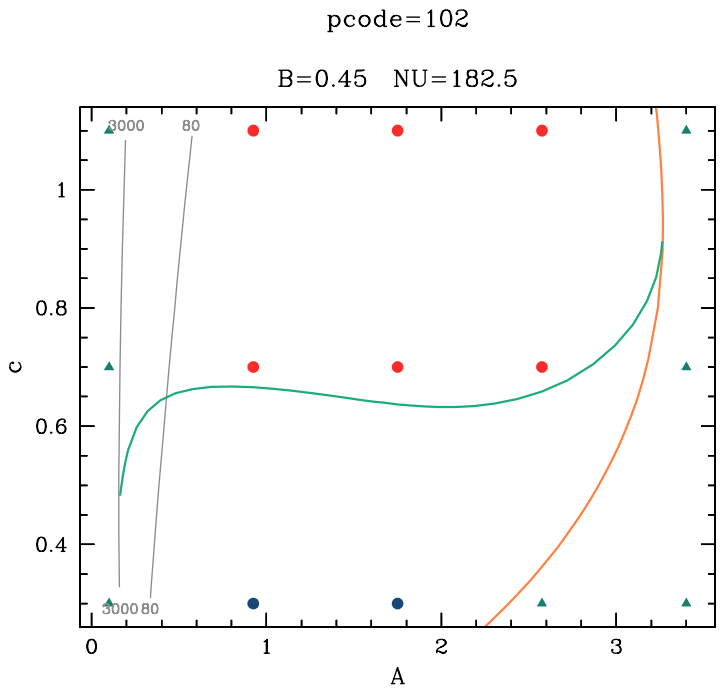


Figure 2.11: A complete plot of the specified part of the control parameter–wave speed plane, for the problem `demo`. A key illustrating the meaning of the various colours and symbols is shown in Figure 2.4 on page 19. The run and plot commands used to generate this figure are given in the main text, and are also listed in the Appendix.

```
@postscript demoplot
```

and then re-enters this series of four plotter commands. However the postscript plot is at this stage only present in a buffer: to complete the file one must either return to screen output via the command `@screen`, or exit the plotter via `@quit` or `@exit`. (Alternatively, one can use the `@postscript` command again to start a new postscript file: this also flushes the output buffer). The plot is then available in the file `demoplot.eps`, in the subdirectory `postscript_files/demo/` of the main WAVETRAIN directory. Recall also that a key showing the meaning of the various dots and lines is given in `pplane_key.eps` in the same subdirectory; the key is illustrated in Figure 2.4. Note that each postscript file generated by WAVETRAIN contains a single plot: there is no capability to produce multi-page postscript files.

2.2 Details of the WAVETRAIN Input Files

For each problem to be studied using WAVETRAIN, the user must create a subdirectory of `input_files` containing the following files:

`constants.input` This file contains computational constants.

`equations.input` This file specifies the equations to be studied.

`other_parameters.input` (*optional*) This file can be used to specify values for parameters other than the control parameter that occur in the model equations. If there are no such parameters, then the file can either be present but empty (apart from any comments) or can be absent.

`parameter_list.input` This file is only required if the user wishes to run the command `add_points_list`; it specifies a list of control parameter and wave speed values to be studied via this command.

`parameter_range.input` This file specifies the range of control parameter and wave speed values to be studied. It also specifies the number of values of each to be used in a parameter grid for the commands `add_points_loop`, `ptw_loop` or `stability_loop`, and these numbers must be present even if the user does not intend to run either of these commands.

`variables.input` This file specifies the names to be used for the various variables.

For the input directories provided as examples in the installation copy of WAVETRAIN, each of these files contains detailed comments explaining their contents.

In fact, not all computational constants are defined in `constants.input`. Rather, this file contains those constants that it is anticipated users will wish to change according to the problem being studied. Remaining constants are contained in the file `defaults.input` in the `input_files` directory itself. It is not expected that users will need to change the constants in `defaults.input` very often, but the file is available to be editted if desired, and again it contains detailed comments explaining the meaning of each constant. The `input_files` directory also contains a number of plotter input files. The file `plotter_defaults.input` contains the default values for a wide range of plotter settings, while files with the extension "`.style`" specify line styles, colours etc. (see §3.3.1). It is not anticipated that new users will want to change these files, but more experienced users may wish to do so, in order to "fine tune" the plots produced by WAVETRAIN. Both `plotter_defaults.input` and the `.style` files contain detailed comments on each entry.

Full details of the files located in the input subdirectory for a particular problem are given below. Details of the `defaults.input` file are given in §3.2, and details of the `.style` files and the file `plotter_defaults.input`, are given in §3.4.

2.2.1 Details of `constants.input`

This file contains those computational constants that are expected to vary according to the problem being studied. Apart from comment lines, the file for the example `demo` is as follows.

```
1 3 # iclean:  1/2=clean/do not, info:  1/2/3/4=log/error/major/all
1 # iwave
30 # nmesh1:  for accurate ptw calc (for ptw period)
```

```
  30 # nmesh2:  for ptw and eigenvalue calculations (< or = nmesh1)
  30 # nmesh3:  for spectrum continuation
  0.005 0.002 0.05 # ds(>0),dsmin,dsmax for locating Hopf bifns
  0.1 0.05 0.5 # ds(>0),dsmin,dsmax for continuation of ptws
  0.001 0.001 0.252 # ds(>0),dsmin,dsmax for continuation of spectrum
  0.2 0.2 1.0 # ds(>0),dsmin,dsmax for stability boundary calcs
  4 1 # nevalues (no. of periodic evalues), iposre (0/1=all/only +ve Im)
  2 # inttype (1=all ptw components, 2=only pde components)
  1 # order:  accuracy order of approx of highest spatial derivative
```

Note that here and in all WAVETRAIN input files, # indicates that the remainder of the line is a comment. The meaning of the various constants is as follows.

`iclean`

WAVETRAIN commands create a variety of temporary files during runs. These are deleted at the end of a run if `iclean`=1, but not if `iclean`=2. Normally `iclean` should be set to 1; the option `iclean`=2 may be useful as a diagnostic tool.

`info`

The level of output information written to the screen is determined by `info`. In all cases, full output information is always written to the file `info.txt` in the relevant output subdirectory. (See §4.4 for a discussion of the output directory structure).

`info`=4: full output information is written to the screen, as well as to `info.txt`.

`info`=3: a subset of information is written to the screen: this provides basic information on the progress of the run.

`info`=2: only error messages are written to the screen, plus an output line indicating the code number allocated to the run.

`info`=1: there is no screen output, and an output line indicating the code number allocated to the run (which is needed for plotting the results) is written to the file `output_files/logfile`.

There two minor exceptions to the above, as follows:

Exception 1: an error may occur that prevents the determination of the value of `info`. For example, there might be a typo in the subdirectory name so that the relevant input subdirectory does not exist. In such a case an error message is written to the screen only.

Exception 2: an error may occur that does not prevent the determination of the value of `info`, but does prevent the creation of the output subdirectory. If `info`=1, an error message is written to `output_files/logfile` as usual in such a case, but if `info`=2, 3 or 4 then an error message is written to the screen only.

For interactive runs it is recommended to set `info`=3 since `info`=4 typically bombards the user will too much information. For background runs it is recommended to set `info`=1.

`iwave`

`iwave`>0 causes the program to select the periodic travelling wave at the `iwave`-th occurrence of the specified value of the control parameter along the solution branch. `iwave`=0 is similar to `iwave`=1 but specifies additionally that, during numerical continuation in the control parameter to search for a Hopf bifurcation in the travelling wave equations, if the specified value of the control parameter is reached before a Hopf bifurcation is detected, then it is assumed that there is no periodic travelling wave for the specified values of the control parameter and wave speed. This has the advantage of eliminating a lot of unnecessary searching for non-existent periodic travelling waves in some cases. It is strongly recommended that when first studying a new problem, `iwave` is set to 1. It is also strongly recommended that `iwave`>1 only be used on the basis of a bifurcation diagram, which can be generated via the command `bifurcation_diagram` (see §3.1.5).

`nmesh1, nmesh2, nmesh3`

The constants `nmesh1`, `nmesh2` and `nmesh2` are the number of mesh intervals used in the discretisation of the solutions, for the three different calculations. These constants are used as the values of the AUTO parameter `ntst`; users familiar with AUTO should note that the AUTO constant `ncol` is set to 4 for all WAVETRAIN computations.

If `nmesh2`<`nmesh1`, then the periodic travelling wave is calculated twice, first for an accurate value of the periodic travelling wave period, and second for the periodic travelling wave used in the eigenvalue calculations. The lower `nmesh2` value is used simply to reduce computation times. If `nmesh2`=`nmesh1` then the periodic travelling wave calculation is done only once. Setting `nmesh2`>`nmesh1` gives an error. It is recommended to set `nmesh1`=`nmesh2` unless a particularly accurate value of the wave period is needed. Note that if `nmesh2` is set to too small a value, then the first continuation run for the spectrum may fail because the approximations to the periodic eigenfunctions and the corresponding eigenvalues are too poor, due to the coarse discretisation (see §3.1.10).

For both periodic travelling wave calculations, the same value of `nmesh` (`nmesh1` for the first calculation and `nmesh2` for the second) is used for both the location of the Hopf bifurcation point in the periodic travelling wave equations, and the continuation of the periodic travelling wave solution from this Hopf bifurcation point. For calculations of Hopf bifurcation loci and contours of constant period, `nmesh2` is used.

The run time for calculating the eigenvalues of the discretised equations (with periodic boundary conditions) increases rapidly with `nmesh2`, which determines the size of the matrix whose eigenvalues are to be calculated. Therefore large values of `nmesh2` should be used only if necessary (see §3.1.10). If `nmesh2` is too small then two problems arise: (i) spurious eigenvalues, due to the discretisation, with no corresponding eigenvalues in the partial differential equation; (ii) poor approximations to the partial differential equation eigenvalues.

Note that the value of `nmesh2` in `constants.input` is not used by the command

eigenvalue_convergence. Instead the various values of nmesh2 specified in the command line are used. However the other parameters set in constants.input do apply.

If nmesh3=nmesh2, so that the number of collocation points in the spectrum continuation is the same as in the calculation of the periodic travelling wave solution, then the periodic travelling wave solution used in the spectrum continuation is simply inherited directly from the calculated solution. However this is not necessary, and AUTO will interpolate to a new mesh as required. Setting nmesh3<nmesh2 is usually desirable to reduce run times; setting nmesh3>nmesh2 is permitted but would rarely be used.

For calculations of stability boundaries, nmesh3 is used.

ds, dsmin, dsmax

These are the initial, minimum and maximum step sizes used in the various numerical continuation calculations. The signs of ds are set appropriately in the relevant programs; they should all be set positive in this file. The appropriate values are highly problem-dependent and some experimentation may be necessary to identify appropriate values. Values that are too small can lead to excessive run times; values that are too large can cause convergence errors or can cause bifurcation points and other critical points to be "jumped over". The first trio of values is used when locating Hopf bifurcations in the periodic travelling wave equations. The second trio of values is used for continuation of branches of periodic travelling wave solutions, including the calculation of bifurcation diagrams and contours of constant period. They are also used for tracing the locus of Hopf bifurcation points in the control parameter–wave speed plane. However, in the calculation of bifurcation diagrams, Hopf bifurcation loci, and contours of constant period, continuations may be done to locate a Hopf bifurcation in the travelling wave equations with the wave speed being the principle continuation parameter rather that the control parameter. (This will occur if the two control parameter values specified in the command arguments are the same, while those for the wave speed are different). Then the ds values used are based on those set in this file (the first trio of values), but with a rescaling. The rescaling is based on the parameter ranges set in parameter_range.input: specifically, all three of ds, dsmin and dsmax are multiplied by the scaling factor (wave_speed_min+wave_speed_max) / (control_param_min+control_param_max). However, the values specified in this file are then used for the subsequent continuations, in which the wave speed and control parameter are both continuation parameters.

The third trio of values is used for continuation along the eigenvalue spectrum. When setting these values, it should be remembered that the principle continuation parameter changes by 2π during each continuation. Therefore it is recommended to set dsmax no larger than about $2\pi/50 = 0.126$ in this case. The fourth trio of values is used for locating and continuing stability boundaries of both Eckhaus and Hopf type. In many cases these can be set to the same values as for periodic travelling wave continuations. However, since these computations are typically rather time-

consuming, larger values should be used if possible. Note that the same step sizes are used to locate the stability boundary whether this is done by varying the control parameter for a fixed wave speed, or vice-versa.

A note for users familiar with AUTO: in the continuations for locating and continuing stability boundaries, derivatives of eigenfunctions are excluded from the pseudo-arclength calculation. Also, in the Eckhaus case, the second derivative of the real part of the eigenvalue with respect to the phase difference across the eigenfunction is excluded, while in the Hopf case, the first derivative of the imaginary part of the eigenvalue with respect to the phase difference is excluded. As a result, it is appropriate to use the same trio of values for both types of stability boundary. However, the pseudo-arclength does include the eigenfunction, the eigenvalue, and the first derivative of the real part of the eigenvalue with respect to the phase difference. This may cause the appropriate step sizes for stability boundary calculations to be different from those for the continuation of periodic travelling wave solution branches.

`nevalues`

The first stage in the calculation of the spectrum is to find eigenvalues for which the eigenfunction is periodic with the period of the wave ("periodic eigenvalues"). The constant `nevalues` specifies the number of these (chosen in order of real part) to be used as starting points for the calculation of the spectrum itself. The issue is that the spectrum may protrude into the right hand half of the complex plane in between two periodic eigenvalues that both have negative real part. In principle this can happen in between any two adjacent periodic eigenvalues, but it is most common for periodic eigenvalues whose real part is almost maximal. Therefore the recommended value of `nevalues` is about 10.

`iposre`

If `iposre`=1 then only eigenvalues with imaginary part greater than or equal to zero are used for output; if `iposre`=0 then all eigenvalues are used for output. The recommended value is `iposre`=1 unless the user is generating a plot of the spectrum for use in publication/presentation.

`inttype`

When calculating stability boundaries, integral conditions are imposed which ensure that the derivatives of the eigenfunction of the periodic travelling wave with respect to $i\gamma$ are orthogonal to the nullspace of the eigenfunction ordinary differential equations. Here γ is the phase difference in the eigenfunction over one period of the periodic travelling wave. These integral conditions can be formulated either in terms of all of the periodic travelling wave components (given by `inttype`=1), or (in most cases) also in terms of just the periodic travelling wave components that correspond to partial differential equation variables (given by `inttype`=2). The recommended value is `inttype`=2 for most problems, which tends to give greater computational reliability (Rademacher *et al.*, 2007). Note that setting `inttype`=2 requires that for each of the partial differential equation variables, there is a direct assignment of one of the periodic travelling wave variable

to that partial differential equation variable. Thus if one of the partial differential equation variables is u, say, then one of the assignments in `variables.input` must be "<`periodic_travelling_wave_variable`>=`u`".

`order`

The first step in calculating the eigenvalue spectrum is to discretise the linearised partial differential equations for eigenfunctions that are periodic with the same period as the periodic travelling wave; here the linearisation is about the periodic travelling wave. This gives a matrix eigenvalue problem which is solved to obtain the periodic eigenfunctions and the corresponding eigenvalues. To do this, spatial derivatives must be converted into finite difference approximations. The constant `order` specifies the order of this approximation for the highest spatial derivative. This determines the number of grid points used to represent the derivative. The approximation is calculated using the algorithm of Fornberg (1998). Since the approximation always uses the same number of grid points on either side of the point at which the derivative is being calculated, the order will actually be one higher than that specified if the number of the highest derivative number is odd, and it may be higher anyway if there are particular symmetries. Usually `order` = 1 is sufficient, and is the recommended value. However higher values may help the accuracy of the approximations to the periodic eigenfunctions and the corresponding eigenvalues, and hence may help if there are difficulties with convergence in the first AUTO run in the calculation of the spectrum. (This run is a continuation in a dummy parameter to locate a solution of the eigenfunction equations, starting from the discretised periodic eigenfunction and corresponding eigenvalue). Examples of the use of `order` > 1 are given in this section (see §2.3.9–2.3.11) and in §3.1.11.

Run times in WAVETRAIN depend strongly on the values of the constants set in the file `constants.input`. Typically run times can be reduced most easily by: (i) decreasing the `nmesh` values, especially `nmesh3`; (ii) increasing `dsmax` for the spectrum continuation; (iii) decreasing `nevalues`, with `iposre` set to 1.

2.2.2 Details of `equations.input`

This file specifies the equations to be studied. For the example `demo`, the file is as follows (apart from some comment lines):

```
# Travelling wave equations
U_z=V
V_z=-c*V-W*U*U+B*U
W_z=(W*U*U+W-A)/(NU+c)
#
# Steady states
A<2.001*B
          none
2.001*B<=A
          U=2*B/(A-sqrt(A^2-4*B^2))
          V=0
          W=(A-sqrt(A^2-4*B^2))/2
```

```
#
# Wave search method and Hopf bifurcation search range
direct # "direct" / "indirect" :  control param / "file"
3.8 # start control param / start speed / soln control param
2.001*B # end control param / end speed / soln speed
#
# Linearised partial differential equations
u_t=
      u_xx  &  1
      u     &  2*U*W-B
      w     &  U^2
w_t=
      w_x   &  NU
      u     &  -2*W*U
      w     &  -1-U**2
#
# The matrix A in the eigenfunction equations
0             &  1   &  0
B-2*U*W       &  -c  &  -U^2
2*U*W/(NU+c)  &  0   &  (1+U**2)/(NU+c)
#
# The matrix B in the eigenfunction equations
0  &  0  &  0
1  &  0  &  0
0  &  0  &  1/(NU+c)
```

WAVETRAIN converts this file into a series of Fortran77 subroutines. Before describing the various sections of this file, a summary is given of the syntax that is used.

Case sensitivity: Names of variables and parameters are case sensitive.

Derivatives: Derivatives are denoted by `_`. For example, for a partial differential equation variable `u`:

if `x` is the space variable then `u_x` denotes du/d`x` and `u_xx` denotes d^2`u`/d`x`^{2};
if `xi` is the space variable then `u_xi` denotes du/d`xi` and `u_xixi` denotes d^2`u`/d`xi`^{2};
if `xx` is the space variable then `u_xx` denotes du/d`xx` and `u_xxxx` denotes d^2`u`/d`xx`^{2}.

(It would be rather pathological to choose `xx` as the space variable, but it would not cause difficulties).

Spaces and blank lines: Spaces and blank lines are allowed and are ignored, but each of the required entries must be on a single line: **line breaks are not allowed**.

Arithmetic:
Powers are denoted by $\wedge$ or $**$
Multiplication is denoted by $*$
Division is denoted by /

Addition is denoted by +
Subtraction is denoted by −
Brackets must be rounded, (and)
Integer division is not allowed. For example (4/3) may be evaluated as 1 (integer part) or 1.333 depending on the context. Therefore 4.0/3.0 should be used instead.

Mathematical functions: The following standard mathematical functions are allowed:

`abs`: absolute value.
`acos`: inverse cosine; result between 0 and π.
`asin`: inverse sine; result between $-\pi/2$ and $\pi/2$.
`atan`: inverse tangent; result between $-\pi/2$ and $\pi/2$.
`cos`: cosine, angle in radians.
`cosh`: hyperbolic cosine.
`exp`: exponential function.
`log`: natural logarithm.
`log10`: base 10 logarithm.
`sin`: sine, angle in radians.
`sinh`: hyperbolic sine.
`sqrt`: square root.
`step1`: step function; result $0, 0, 1$ for argument $< 0, = 0, > 0$.
`step2`: step function; result $0, 0.5, 1$ for argument $< 0, = 0, > 0$.
`step3`: step function; result $0, 1, 1$ for argument $< 0, = 0, > 0$.
`tan`: tangent, angle in radians.
`tanh`: hyperbolic tangent.

Either upper or lower case can be used for these functions: for example `abs`, `Abs` and `ABS` are equivalent. Note that square roots can be denoted either by `^0.5` or `sqrt` (or `Sqrt` or `SQRT`).

It would be rather confusing to use one of these function names as a variable name, but it is permitted: the conversion to Fortran77 can distinguish between the use of these names as functions, when they must be followed by a left bracket "`(`", and as variable names, when they cannot be followed by a left bracket.

Comments: The hash symbol (#) is used to indicate a comment. Any part of a line after a # is ignored.

Having established the syntax, the various sections of the file are now described, in order. Note that it is essential that the sections are given in the correct order.

Travelling wave equations: These are specified using the syntax described above, and using the travelling wave variables and travelling wave coordinate given in the file `variables.input`.

Steady states: Periodic travelling waves typically develop from a Hopf bifurcation of a steady state solution of the travelling wave equations. In simple cases, this steady state can be specified by a single formula for each travelling wave variable, valid for all values of the control parameter being considered. More generally, the steady state will exist only for some parameter values. Therefore the steady state solution is specified via a series of conditions on parameter values, each of which is followed either by a list of the steady states (using travelling wave variables), or by the single word `none` (or `None` or `NONE`). The parameter conditions must cover all possible values of the control parameter, and must consist of inequalities written using `<`, `>`, `<=` and `>=`. Multiple inequalities must be written as single inequalities separated by `&` (double-sided inequalities are not allowed).

In some cases an exact formula will not be available for the steady state. This is not a problem if a formula for a suitable approximation can be given, since the steady state formulae given in `equations.input` are not used directly: rather, they are used as an initial guess for a numerical calculation of the steady states. However it is often not possible to provide a suitable approximation as a function of parameters. In this case, the user must enter the single word `file` (or `File` or `FILE`), and must provide an additional input file called `steadystate.input` (in the appropriate input subdirectory). This file should contain a series of control parameter values and associated steady state information, which must be generated by some other computer program. The required format is:

column 1: control parameter value

column 2: 0 or 1, indicating that a steady state does not or does exist

remaining columns, if 1 in column 2: the steady state values, given for the same ordering of the periodic travelling wave variables as in `variables.input`.

The control parameter values must appear in either increasing or decreasing order. This file is read in and then for any specified value of the control parameter, a steady state is estimated by linear interpolation, and then refined via numerical calculation of the steady states. Therefore the control parameter values in `steadystate.input` must span the entire range of values being considered. The interpolation is conservative with respect to steady state existence: if a steady state does not exist for either of the two control parameter values straddling the specified value, then it is assumed not to exist. The problem `demo3`, discussed in §3.1.11, illustrates the provision of the steady state via a user-supplied file. Note that if the "file" wave search method (see below) is used for all control parameter and wave speed values, then the steady states are not used. However a dummy specification is still required; this can be "file", and then no `steadystate.input` file is needed.

A common situation is that the steady state exists only on one side of a parameter threshold, with a saddle-node bifurcation at the threshold. In this case, there will be two steady states on one side of the threshold, only one of which is of interest (in any particular run). If the exact saddle-node point is specified in the parameter inequalities, then it is quite possible that, starting from this saddle-node point,

WAVETRAIN will numerically continue the steady state along the wrong steady state branch. To avoid this, the user is strongly recommended to define the steady state as not existing for parameter values very close to the threshold.

Wave search method and Hopf bifurcation search range: Typically, periodic travelling waves develop from a Hopf bifurcation of the steady state specified in the previous part of `equations.input`. The next part of the file specifies the method used to search for periodic travelling waves, and the associated range of parameters used to search for the initial Hopf bifurcation point. Three methods are available. Typically, periodic travelling waves develop from a Hopf bifurcation of the steady state specified in the previous part of this input file, and two of these methods involve first locating a Hopf bifurcation in the steady state. These methods are termed "direct" and "indirect" because after detecting the Hopf bifurcation, WAVETRAIN locates the periodic travelling wave in either one or two steps, respectively. The third available method is termed "file", and does not involve locating a Hopf bifurcation point. Rather, the user is required to provide a periodic travelling wave solution for one pair of control parameter and wave speed values (e.g. from simulations of the partial differential equations). This solution is then used as a starting point for calculating wave solutions for other control parameter and wave speed values.

Direct method: In this case the user specifies a search range of control parameter values. WAVETRAIN will then search this range for a Hopf bifurcation in the travelling wave equations, with the wave speed fixed at the value for which a periodic travelling wave is sought. Having found a Hopf bifurcation, WAVETRAIN then tracks the branch of periodic travelling waves as the control parameter varies, again with fixed wave speed, until the required control parameter value is reached.

Indirect method: In this case the user specifies a search range of wave speed values, and a control parameter value for the search. WAVETRAIN will then search for a Hopf bifurcation on this basis. Having found a Hopf bifurcation, it will first track the branch of periodic travelling waves as the wave speed varies, with the control parameter fixed at the value specified for the Hopf bifurcation search, until the required wave speed is reached. WAVETRAIN then fixes the wave speed at this value and tracks the periodic travelling waves as the control parameter is varied, until the required value is reached.

File method: In this the user specifies a pair of control parameter and wave speed values, and provides an additional input file `ptwsoln.input` that contains the solution for these parameter values. The file must be placed in the relevant input subdirectory. Using this solution as a starting point, WAVETRAIN will first track the branch of periodic travelling waves as the wave speed varies, with the control parameter fixed at the value specified for the Hopf bifurcation search, until the required wave speed is reached. WAVETRAIN then fixes the wave speed at this value and tracks the periodic travelling waves as the control parameter is varied, until the required value is reached. The required format for the file `ptwsoln.input` is:

column 1: travelling wave (or space) coordinate

remaining columns: the travelling wave variables, in the same order as listed in `variables.input`.

There are no particular constraints on the discretisation used for the solution in the file. It must be given over one period of the periodic travelling wave, and the travelling wave variable values given in the last line must be exactly the same as those given in the first line. The corresponding space/travelling wave coordinate with then be one period greater than that in the first line: usually this coordinate will be an approximation, found by linear interpolation.

In simple cases a single method will be specified for all control parameter and wave speed values, but the choice and details of the method can be parameter dependent, specified using inequalities with the same syntax as described above for steady states. Thus the parameter conditions (which must cover all values of the control parameter and wave speed being studied) must consist of inequalities written using `<`, `>`, `<=` and `>=`. Multiple inequalities must be written as single inequalities separated by `&` (double-sided inequalities are not allowed). The following points should be noted in connection with the specification of the wave search method and Hopf bifurcation search range:

1. (direct and indirect cases) The start value(s) of control parameter/wave speed can be either less than or greater than the end value(s).
2. (direct and indirect cases) The steady state must exist throughout the search range(s).
3. (direct and indirect cases) The start and end values can depend on the control parameter and/or the wave speed.
4. (direct and indirect cases) Choosing range limits that are closer together (and thus closer to the Hopf bifurcation point) will speed up execution.
5. The setting `iwave`=0 (§3.1.8) is only permissible if the search method(s) is/are direct. Then the end value of the search range (for the control parameter) is not used, although a (dummy) value must still be given; it is replaced by the value of the control parameter at which a periodic travelling wave is sought. (This is the only difference between `iwave`=0 and `iwave`=1).
6. The start and end values of the search range (direct and indirect cases) and the specific control parameter and wave speed value (file case) can lie outside the limits specified in `parameter_range.input`.
7. (direct and indirect cases) The Hopf bifurcation search range that is specified in `equations.input` is not used by either the `hopf_locus` command or the `bifurcation_diagram` command. In the former case, the search range is specified in the command arguments, and for the `bifurcation_diagram` command the limits specified in the file `parameter_range.input` are used to search for Hopf bifurcations.
8. (indirect case) Note the semi-colon after the word `indirect`, which is essential.

Linearised partial differential equations: The first step in the calculation of the eigenvalue spectrum is to calculate the eigenvalues corresponding to eigenfunctions that are periodic with the same period as the travelling wave solution. To do this, one first linearises the partial differential equations around the periodic travelling wave solution, and then discretises this in space to give a matrix eigenvalue problem. The discretisation is done automatically by WAVETRAIN, but the linearised partial differential equations must be specified. If the time variable is `t`, the partial differential equation variables are `u`, `v`, `w`,... and the periodic travelling wave variables are `U`, `V`, `W`,... (say), then each linearised equation will have either `u_t`, `v_t`, `w_t`,... or `0` on the left hand side of the equation, and a series of terms on the right hand side, each of which contains exactly one of `u`, `v`, `w`,... or a spatial derivative of one of these partial differential equation variables. The required format for inputting these equations is `u_t=` (or `v_t=` or `w_t=` or ...) or `0=` on a separate line, and then on subsequent lines the partial differential equation variable or its derivative, followed by &, and then the coefficient of this partial differential equation variable/derivative. Each pair of partial differential equation variable/derivative and coefficient must be on a separate line. The coefficients must involve just parameters and travelling wave variables, not the derivatives of travelling wave variables. (If such derivatives arise when the partial differential equations are linearised, these can always be expressed in terms of other travelling wave variables). Note that the equations should be given in terms of the space variable, rather than the travelling wave coordinate. They are converted to a moving reference frame before being discretised.

Eigenfunction equations: Investigation of the stability of periodic travelling waves requires solution of the eigenfunction equations that govern behaviour close to the wave solution. These can be specified by two NPTW × NPTW matrices (where NPTW is the number of travelling wave variables). To derive these matrices it will be necessary to do a few lines of mathematics on a piece of paper, but this should not be difficult or time-consuming. The procedure is as follows:

Step 1: Linearise the partial differential equations about the periodic travelling wave solution, which has been done for the previous part of `equations.input`. The result of this calculation is a linear system of partial differential equations given above. To fix notation, denote the linearised partial differential equation variables by the NPDE-dimensional vector $\underline{u}_{lin}(\mathtt{x},\mathtt{t})$. Here `x` and `t` are the space and time variables, and NPDE is the number of partial differential equation variables.

Step 2: Substitute the solution form $\underline{u}_{lin}(\mathtt{x},\mathtt{t}) = \underline{U}_{lin}(\mathtt{z})\exp(\lambda\mathtt{t})$ where `z=x−ct` is the travelling wave variable with `c` denoting the wave speed. This gives a linear system of ordinary differential equations for $\underline{U}_{lin}$, whose coefficients depend on the travelling wave solution.

Step 3: Typically this linear system of ordinary differential equations will involve second and/or higher order derivatives of $\underline{U}_{lin}$. In the file `variables.input`, the user is required to provide formulae for converting the partial differential equation variables into travelling wave variables. To be specific, denote these

formulae by $\underline{u}_{tw} = F(\underline{u}_{pde}, \partial\underline{u}_{pde}/\partial\mathtt{x}, \partial^2\underline{u}_{pde}/\partial\mathtt{x}^2, \ldots)$. Then the corresponding formulae $\underline{U}_{lin,tw} = F(\underline{U}_{lin}, \partial\underline{U}_{lin}/\partial\mathtt{z}, \partial^2\underline{U}_{lin}/\partial\mathtt{z}^2, \ldots)$ should be used to convert the linear ordinary differential equations into a first order system of ordinary differential equations for $\underline{U}_{lin,tw}$. **Important note:** it is essential that the components of the vector $\underline{U}_{lin,tw}$ are kept in the order corresponding to the order in which the travelling wave variables are listed in the file `variables.input`.

Step 4: The resulting first order linear system of differential equations will always have the form $\partial\underline{U}_{lin,tw}/\partial\mathtt{z} = A\,\underline{U}_{lin,tw} + \lambda\,B\,\underline{U}_{lin,tw}$ where A and B are NPTW $\times$ NPTW matrices.

The final two sections of the file specify the matrices A and B, with columns separated by ampersands (`&`).

2.2.3 Details of `other_parameters.input`

This file can be used to specify values for parameters other than the control parameter that occur in the model equations. Apart from comment lines, the file for the example `demo` is as follows.

```
B=0.45      # <name> = <value>
NU=182.5
```

Spaces and comments (indicated by #) can be included in this file if desired: they will simply be ignored. Note that if the partial differential equations being studied do not contain any parameters other than the control parameter then this file can either be absent, or can exist but be empty, or can exist but have only comment lines.

2.2.4 Details of `parameter_list.input`

This file is only required if the user wishes to run the `add_points_list` command; it specifies a list of control parameter and wave speed values to be studied via this command. Apart from comment lines, the file for the example `demo` is as follows.

```
2.0 0.61
2.0 0.65
```

The first column are control parameter values and the second column are wave speed values. For each pair of values, the command `add_points_list` calculates the periodic travelling wave; stability is also calculated if the `pcode` value in the argument list was generated using the `stability_loop` command. Note that the axes limits in control parameter–wave speed plots are based on the entries in the file `parameter_range.input` at the time of the initial run of `ptw_loop` or `stability_loop`, and are unaffected by runs of `add_points_list`.

2.2.5 Details of `parameter_range.input`

This file specifies the range of control parameter and wave speed values to be studied. It also specifies the number of values of each to be used in a parameter grid for the commands `add_points_loop`, `ptw_loop` or `stability_loop`, and the numbers must be present even if the user does not intend to run any of these commands. Apart from comment lines, the file for the example `demo` is as follows.

```
0.1 3.4 3 # min,max,ngrid for control parameter
0.3 1.1 2 # min,max,ngrid for wave speed
```

The specified maximum and minimum values are inclusive. The file is also used when calculating bifurcation diagrams, providing diagram limits for whichever of the control parameter or wave speed is the bifurcation parameter.

2.2.6 Details of `variables.input`

This file specifies the names to be used for the various variables. It contains comments that explain what the various lines denote. For the example `demo`, the file is as follows (apart from some explanatory comments):

```
# variables.input
################################################################
A # NAME FOR THE CONTROL PARAMETER
c # NAME FOR THE WAVE SPEED
x # NAME FOR THE SPACE COORDINATE
t # NAME FOR THE TIME COORDINATE
z # NAME FOR THE TRAVELLING WAVE COORDINATE
################################################################
# PDE VARIABLE NAMES, ONE PER LINE
u
w
################################################################
# TW VARIABLE NAME = FUNCTION OF PDE VARIABLES, ONE PER LINE
U = u
V = u_x
W = w
```

It is essential that the various lines in this file are given in the correct order. Spaces, blank lines and comments (indicated by #) are ignored.

2.3 A Worked Example

Together, §2.1 and §2.2 describe the basic operation of WAVETRAIN, and the details of most of the input files. A number of details of the commands have not been discussed, and a few WAVETRAIN commands have not been mentioned at all; these are considered in §3.1. Before this, I present a full worked example, illustrating how WAVETRAIN can be used to study periodic travelling wave solutions in practice. The example is based on the work of Smith & Sherratt (2007), and concerns the following model for a predator-prey

interaction:

$$\frac{\partial u}{\partial t} = e^{\delta}\frac{\partial^2 u}{\partial x^2} + u(1-u) - \frac{uv}{u+k} \tag{2.1a}$$

$$\frac{\partial v}{\partial t} = e^{-\delta}\frac{\partial^2 v}{\partial x^2} + \frac{suv}{u+k} - \mu v\,. \tag{2.1b}$$

Here u and v denote prey and predator densities respectively, x and t are the space and time coordinates respectively, and k, s, μ and δ are positive parameters. Based on the numerical simulations of (2.1) (see Smith & Sherratt, 2007), the objective is to investigate the existence and stability of periodic travelling waves for the parameter δ in the range $-2 < \delta < 2$, with wave speeds between 0.1 and 4, and with the other three parameters fixed at $k = 0.2$, $s = 0.15$ and $\mu = 0.05$. Note that periodic travelling waves do exist for wave speeds between 0.1 and 0, and these can be investigated using WAVETRAIN. However the computations become significantly more difficult as the speed approaches zero, requiring very small continuation step sizes, which leads to rather long run times.

For ease of presentation, the study is broken up into a number of stages, some involving the creation or replacement of input files, and others involving runs of WAVETRAIN commands. Deliberately, the installation files do not include an input subdirectory corresponding to this example. This is because the example is intended to illustrate all of the stages involved in a WAVETRAIN study, which includes the creation of an input subdirectory. Users may which to perform each stage of this example manually, to help familiarise themselves with the use of WAVETRAIN. However, as an alternative, the command `set_worked_example_inputs` is provided. This command takes as an argument the number of a stage of the study involving input file creation/replacement. It first empties the `workedex` input subdirectory, and then performs all of the steps involved in each of the input stages, in order, up to and including the specified stage. Thus for example the command

```
set_worked_example_inputs 5
```

will first empty the `workedex` input subdirectory, if it exists, and will then perform the various steps in Stage 1, then Stage 3, and finally Stage 5.

2.3.1 Stage 1 (Input): Create the Initial Input Files

The command "`set_worked_example_inputs 1`" *performs all of the steps described in this stage of the study.*

2.3.1.1 Create the Input Subdirectory

The very first step in any WAVETRAIN study is to choose a problem name and create the input directory. There is no constraint on the length of the name, although names with more than 10 characters are abbreviated in screen output. In this case, the name "workedex" seems appropriate, and the input directory is created by the command

```
mkdir input_files/workedex
```

which must be entered from the main WAVETRAIN directory. At installation, a dummy set of input files is provided in the input directory `template`, and this should be copied into the new input directory via the command

```
cp input_files/template/*  input_files/workedex/.
```

(for the benefit of users unfamiliar with unix/linux, it may be helpful to explain that the final dot in this command indicates that the files should be given the same names in the new directory as in `template`).

2.3.1.2 Create the File `equations.input`

To create an initial version of `equations.input`, the various parts of the file should be completed in the order described in §2.2.2, beginning with the travelling wave equations. Substituting $u(x,t) = U(z)$ and $v(x,t) = V(z)$ with $z = x - ct$ into (2.1) gives

$$\begin{aligned} e^{\delta}U'' + cU' + U(1-U) - UV/(U+k) &= 0 \\ e^{-\delta}V'' + cV' + sUV/(U+k) - \mu V &= 0 \end{aligned}$$

where prime denotes d/dz. This must be rewritten as a system of first order equations:

$$\begin{aligned} U' &= P && \text{(2.2a)} \\ P' &= e^{-\delta}\left[-cP - U(1-U) + UV/(U+k)\right] && \text{(2.2b)} \\ V' &= Q && \text{(2.2c)} \\ Q' &= e^{\delta}\left[-cQ - sUV/(U+k) + \mu V\right]. && \text{(2.2d)} \end{aligned}$$

Setting the left hand sides of (2.2) to zero provides a system of algebraic equations that can easily be solved for the unique steady state with U and V both non-zero:

$$U_s = \mu k/(s-\mu) \quad P_s = 0 \quad V_s = (1-U_s)(U_s+k) \quad Q_s = 0\,. \tag{2.3}$$

After calculating the travelling wave equations and steady state, the next part of `equations.input` concerns the wave search method. At this stage no information is available on which this can be based, and therefore the dummy entries provided in the version of the file in the `template` directory should be retained. Note that dummy entries are essential: a blank entry is not permitted.

Moving on to the linearised partial differential equations, these are given by linearising (2.1) about the travelling wave solution $u(x,t) = U(z)$, $v(x,t) = V(z)$, giving

$$\begin{aligned} \frac{\partial u_{lin}}{\partial t} &= e^{\delta}\frac{\partial^2 u_{lin}}{\partial x^2} + u_{lin}\left[1 - 2U - \frac{kV}{(U+k)^2}\right] + v_{lin}\left[\frac{-U}{U+k}\right] && \text{(2.4a)} \\ \frac{\partial v_{lin}}{\partial t} &= e^{-\delta}\frac{\partial^2 v_{lin}}{\partial x^2} + u_{lin}\left[\frac{skV}{(U+k)^2}\right] + v_{lin}\left[\frac{sU}{U+k} - \mu\right] && \text{(2.4b)} \end{aligned}$$

where $u_{lin}(x,t) = u(x,t) - U(z)$ and $v_{lin}(x,t) = v(x,t) - V(z)$, and nonlinear terms have been neglected.

Finally, it is necessary to calculate the matrices A and B in the eigenfunction equations, via the method described in §2.2.2. Substituting $u_{lin}(x,t) = U_{lin}(z)e^{\lambda t}$ into (2.4) gives

$$\begin{aligned}
\lambda U_{lin} &= e^{\delta}\frac{d^2U_{lin}}{dz^2} + c\frac{dU_{lin}}{dz} + U_{lin}\left[1 - 2U - \frac{kV}{(U+k)^2}\right] + V_{lin}\left[\frac{-U}{U+k}\right] \\
\lambda V_{lin} &= e^{-\delta}\frac{d^2V_{lin}}{dz^2} + c\frac{dV_{lin}}{dz} + U_{lin}\left[\frac{skV}{(U+k)^2}\right] + V_{lin}\left[\frac{sU}{U+k} - \mu\right].
\end{aligned}$$

Substituting

$$U_{lin} = U_{lin,tw} \quad dU_{lin}/dz = P_{lin,tw} \quad V_{lin} = V_{lin,tw} \quad dV_{lin}/dz = Q_{lin,tw} \tag{2.5}$$

gives a system of the required form

$$\frac{d}{dz}\begin{bmatrix} U_{lin,tw} \\ P_{lin,tw} \\ V_{lin,tw} \\ Q_{lin,tw} \end{bmatrix} = (A + \lambda B)\begin{bmatrix} U_{lin,tw} \\ P_{lin,tw} \\ V_{lin,tw} \\ Q_{lin,tw} \end{bmatrix}$$

where A and B are the 4×4 matrices

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 \\ e^{-\delta}\left(2U + \dfrac{kV}{(U+k)^2} - 1\right) & -e^{-\delta}c & e^{-\delta}\dfrac{U}{U+k} & 0 \\ 0 & 0 & 0 & 1 \\ -e^{\delta}\dfrac{skV}{(U+k)^2} & 0 & e^{\delta}\left(\mu - \dfrac{sU}{U+k}\right) & -e^{\delta}c \end{bmatrix} \tag{2.6a}$$

$$B = \begin{bmatrix} 0 & 0 & 0 & 0 \\ e^{-\delta} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & e^{\delta} & 0 \end{bmatrix}. \tag{2.6b}$$

Equations (2.2), (2.3), (2.4) and (2.6) must be entered in the `equations.input` file, using the format described in §2.2.2, and also in the comments at the end of the file. Apart from explanatory comments at the end, the resulting file is as follows:

```
# equations.input
#################################################################
# Travelling wave equations
U_z=P
P_z=exp(-delta)*(-c*P-U*(1-U)+U*V/(U+k))
V_z=Q
Q_z=exp(delta)*(-c*Q-s*U*V/(U+k)+mu*V)
#################################################################
# Steady states
U=mu*k/(s-mu)
P=0
V=(1-(mu*k/(s-mu)))*((mu*k/(s-mu))+k)
```

```
Q=0
################################################################
# Wave search method and Hopf bifurcation search range
direct # "direct" / "indirect" :  control param / "file"
0.0 # start control param / start speed / soln control param
0.0 # end control param / end speed / soln speed
################################################################
# Linearised partial differential equations
u_t=
     u_xx & exp(delta)
     u & 1-2*U-k*V/((U+k)**2)
     v & -U/(U+k)
v_t=
     v_xx & exp(-delta)
     u & s*k*V/((U+k)**2)
     v & s*U/(U+k)-mu
################################################################
# The matrix A in the eigenfunction equations
0 & 1 & 0 & 0
exp(-delta)*(2*U+k*V/((U+k)**2)-1) & -exp(-delta)*c & exp(-delta)*U/(U+k) & 0
0 & 0 & 0 & 1
-exp(delta)*s*k*V/((U+k)**2) & 0 & exp(delta)*(mu-s*U/(U+k)) & -exp(delta)*c
################################################################
# The matrix B in the eigenfunction equations
0 & 0 & 0 & 0
exp(-delta) & 0 & 0 & 0
0 & 0 & 0 & 0
0 & 0 & exp(delta) & 0
```

Note that although two of the rows of the matrix A cause rather long lines, they must be entered on a single line: line breaks are not permitted in `equations.input`.

2.3.1.3 Create the File `variables.input`

The various parts of `variables.input` must now be completed, giving the file as follows (apart from the explanatory comments at the end of the file):

```
# variables.input
################################################################
delta   # NAME FOR THE CONTROL PARAMETER
c       # NAME FOR THE WAVE SPEED
x       # NAME FOR THE SPACE COORDINATE
t       # NAME FOR THE TIME COORDINATE
z       # NAME FOR THE TRAVELLING WAVE COORDINATE
################################################################
# PDE VARIABLE NAMES, ONE PER LINE
u
v
################################################################
# TW VARIABLE NAME = FUNCTION OF PDE VARIABLES, ONE PER LINE
U = u
P = u_x
V = v
Q = v_x
```

Note that it is essential that the order in which the travelling wave variables are listed corresponds to the order used for the matrices A and B in `equations.input`.

2.3.1.4 Create the File `other_parameters.input`

This file is simply a listing of the parameters other than the control parameter, and their required values. Apart from explanatory comments at the end, the file is:

```
k=0.2 # <name> = <value>
s=0.15
mu=0.05
```

2.3.1.5 Create the File `parameter_range.input`

This file specifies the range of control parameter (δ) and wave speed (c) values to be considered. It also specifies the numbers of grid points used for scans of the control parameter – wave speed plane. This latter information is not needed at this stage, but it is convenient to enter appropriate values, to save changing the file later: an 8×8 grid is suitable, and would be an appropriate initial choice for many problems. Apart from explanatory comments at the end, the file is therefore:

```
 -2 2 8 # min,max,ngrid for control parameter
0.1 4 8 # min,max,ngrid for wave speed
```

2.3.1.6 Create the File `constants.input`

In the directory `template`, the various entries in `constants.input` are given values that are good starting points for many problems. Note that the entries are different from those used for the problem `demo`, which were effective for demonstration purposes but would not be suitable for many real problems. Therefore at this stage, the version of `constants.input` that has been copied from the `template` directory can be used without changes.

2.3.2 Stage 2 (Run): Formulate a Wave Search Method

The input files generated in Stage 1 lack one key ingredient: a wave search method was not specified in `equations.input`. The key tool for formulating a method is the `hopf_locus` command, which does not use the wave search method part of `equations.input`. However, this command requires a pcode value as one of its arguments. In §2.1, `hopf_locus` was run after a run of `ptw_loop` or `stability_loop` so that a pcode value was available, but that is not the case here. The WAVETRAIN command `new_pcode` is provided for this purpose. This command will be described in §3.1.4, but it is very simple. It takes only one argument, the input directory name, sets up a blank control parameter – wave speed plane, and allocates a pcode value. Therefore, to begin investigation of the `workedex` problem, one types

```
new_pcode workedex
```

and WAVETRAIN reports that the allocated pcode value is 101.

The `hopf_locus` command can now be run. In the absence of any information about control parameter and wave speed values for which the travelling wave equations might have a Hopf bifurcation, it is necessary to experiment blindly. Typing

```
hopf_locus workedex 101 -1 0 -1 6
```

causes WAVETRAIN to report that it did not detect a Hopf bifurcation in the range $0 < c < 6$ for $\delta = -1$. Note that the range of c being investigated by the command is wider than the range specified in `parameter_range.input`, which is permitted. Note also that the run is allocated an hcode value even though it is unsuccessful. As a second attempt, type

```
hopf_locus workedex 101 1 0 1 6
```

which does successfully locate a Hopf bifurcation and trace its locus. To plot this, start the plotter by typing

```
plot workedex 101
```

and plot the locus by entering first

```
@pplane
```

and then

```
@hopf_locus 102
```

at the plotter prompt. (Here 102 is the hcode value of the successful run). The resulting plot is shown in Figure 2.12.

2.3.3 Stage 3 (Input): Add a Preliminary Wave Search Method

The command "`set_worked_example_inputs 3`" performs the steps described in Stage 1 of the study, and then performs the steps described in this stage.

From the plot of the Hopf bifurcation locus in Figure 2.12 one cannot tell whether periodic travelling waves exist for parameters above or below the locus. Indeed it is possible that both of these possibilities apply, because of folds in the periodic travelling wave solution branches. In fact, numerical simulations of the partial differential equations (Smith & Sherratt, 2007) suggest that waves exist only above the locus, but this can be determined using WAVETRAIN, without *a priori* knowledge. To do this, one must formulate a preliminary wave search method that will apply for $0.1 < c < 1.0$; this will be amended to cover larger values of c in Stage 5. There is a Hopf bifurcation in the travelling wave equations for every value of c between 0.1 and 1, with the corresponding value of δ lying between -1 and 2. Therefore the file `equations.input` can be editted, replacing the dummy wave search method with

```
# Wave search method and Hopf bifurcation search range
direct # "direct" / "indirect" :  control param / "file"
-1.2 # start control param / start speed / soln control param
2.2 # end control param / end speed / soln speed
```

Note that the search range has been set slightly wider than strictly necessary; this is good practice to avoid problems due to large jumps in the first few continuation steps.

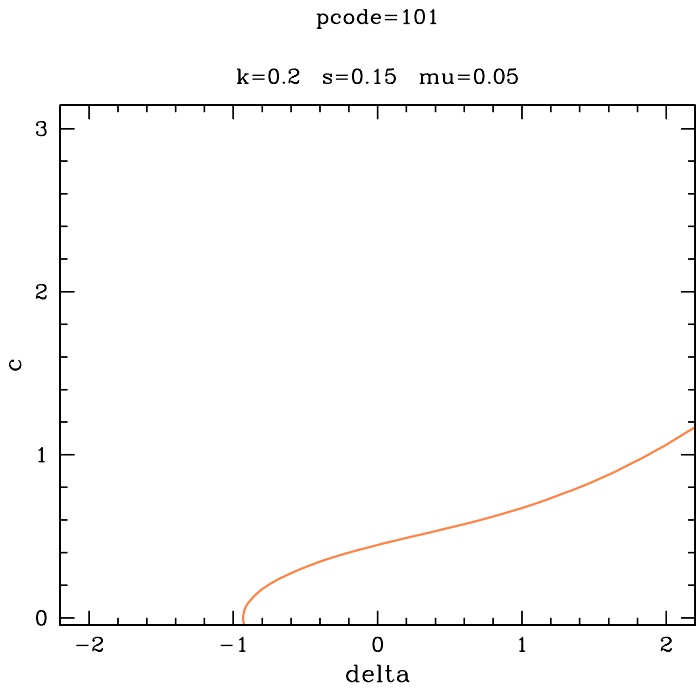


Figure 2.12: A plot of the locus of Hopf bifurcation points in the control parameter–wave speed plane, for the worked example problem `workedex`. The run and plot commands used to generate this figure are given in the main text, and are also listed in the Appendix.

2.3.4 Stage 4 (Run): Look for Waves near the Hopf Bifurcation Locus

With the preliminary wave search method in place, one can look for periodic travelling waves on either side of the Hopf bifurcation locus. For example, the run

```
ptw workedex 0 0.7
```

successfully detects a periodic travelling wave, while

```
ptw workedex 1.0 0.3
```

fails to find a wave solution. Based on this and other similar runs (which must have c between 0.1 and 1) one can draw the (tentative) conclusion that close to the Hopf bifurcation locus, waves exist above the locus and not below.

2.3.5 Stage 5 (Input): Amend the Wave Search Method

The command "`set_worked_example_inputs 5`*" performs the steps described in the previous input stages of the study, and then performs the steps described in this stage.*

Based on the results of Stage 4, it is now necessary to amend the wave search method to cover all points in the parameter plane under study that lie above the Hopf bifurcation locus. One possible approach to this would be to calculate the Hopf bifurcation locus over a large range of δ values. Depending on the shape of the locus, it might then be possible to formulate a single direct search method: note that parameter ranges used in the wave search method can be wider than those specified in `parameter_range.input`. However, it is simpler to formulate a mixed search method based only on the results in Figure 2.12. An appropriate choice is:

```
# Wave search method and Hopf bifurcation search range
c<=1
     direct # "direct" / "indirect" :  control param / "file"
     -1.2 # start control param / start speed / soln control param
     2.2 # end control param / end speed / soln speed
c>1
     indirect :  0.0 # "direct" / "indirect" :  control param / "file"
     0.0 # start control param / start speed / soln control param
     0.9 # end control param / end speed / soln speed
```

Note that there is nothing special about the choice of 0.0 as the fixed value of δ for the Hopf bifurcation search in the indirect case.

2.3.6 Stage 6 (Run): Test Runs of the `ptw` Command

Having set up the wave search method, it is necessary to test the `ptw` command at a number of control parameter and wave speed values. The objective is to check whether the computational constants set in `constants.input` (and potentially also in `defaults.input`) are suitable for this problem. As examples, the commands

```
ptw workedex 1.5 2.5
ptw workedex 2.0 1.2
ptw workedex 0.5 4.0
ptw workedex -1.0 0.7
ptw workedex -2.0 0.2
```

all successfully find periodic travelling waves. In the third case a warning is reported about a small number of continuation steps. This is because $\delta = 0.5$ is rather close to the value fixed for the Hopf bifurcation search ($\delta = 0$), and the warning is not a cause for concern. However, the command

```
ptw workedex -1.5 0.1
```

unexpectedly fails to find a travelling wave, due to a convergence problem during the periodic travelling wave continuation. As explained in the screen output, this type of error commonly occurs because the wave solution branch is approaching a homoclinic solution. (An example of this is provided by the problem `demo` discussed in §2.1). However the warning message that only two continuation steps were taken strongly suggests that a real convergence error has occurred. Users with previous experience with AUTO may find it valuable to look at the `info.txt` file associated with the run in a situation such as this; `info.txt` contains the full output from AUTO (see §2.5 for details).

2.3.7 Stage 7 (Input): Alter the File `constants.input`

The command "`set_worked_example_inputs 7`" *performs the steps described in the previous input stages of the study, and then performs the steps described in this stage.*

There are two likely remedies for a convergence error such as that encountered in Stage 6: either an increase in the values of `nmesh1` and `nmesh2`, or a decrease in the values of `ds` and `dsmin`. Experimentation shows that increasing `nmesh1` and `nmesh2` (keeping them equal for convenience) does not eliminate the error, but reducing `ds` and `dsmin` does. Therefore line 7 of `constants.input` should be altered, with appropriate new settings being

```
0.01 0.01 0.5 # ds(>0),dsmin,dsmax for continuation of ptws
```

2.3.8 Stage 8 (Run): Further Test Runs of `ptw`, and a Run of `ptw_loop`

Further test runs of `ptw` with the amended version of `constants.input` are now necessary. These successfully find periodic travelling waves at all points above the Hopf bifurcation locus in the control parameter – wave speed plane. Therefore one can move on to a systematic loop across the plane, checking for wave existence. The number of grid points to consider was set (in `parameter_range.input`) in Stage 1. Thus one can proceed immediately, via the command

```
ptw_loop workedex
```

which completes the loop without any errors; there are a number of warnings about small numbers of continuation steps, but none of these is significant. Before plotting, it is helpful to recreate the Hopf bifurcation locus shown in Figure 2.12 for this new pcode value, using the command

```
hopf_locus workedex 102 1 0 1 6
```

(alternatively the `copy_hopf_loci` command could be used, although this would also copy across the unsuccessful attempt at $\delta = -1$). After this the plotter can be started by typing

```
plot workedex 102
```

and the results of the `ptw_loop` calculation can be shown by typing

```
@pplane
```

at the plotter prompt, selecting the default plot type. To superimpose the Hopf bifurcation locus, one types

```
@hopf_locus 102
```

giving the plot illustrated in Figure 2.13. This shows that there are periodic travelling waves at all points in the control parameter–wave speed plane above and to the left of the Hopf bifurcation locus. Although it is not necessary, one might be interested to see the form of one or more of these waves. For example, typing

```
@ptw 1037
```

gives a plot of the solution with rcode value 1037, which is shown in Figure 2.14. The point in the δ–c plane to which this corresponds can be seen in Figure 2.13.

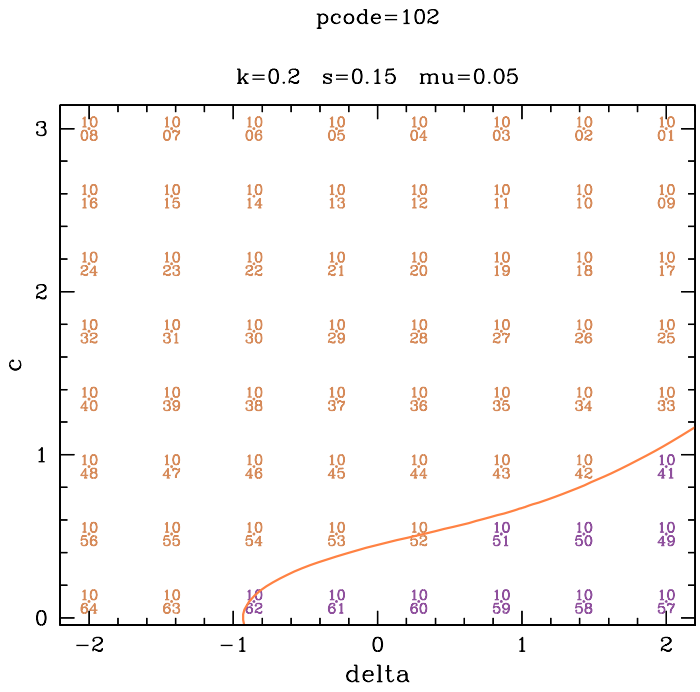


Figure 2.13: Results on the existence of periodic travelling wave solutions for the problem `workedex`. A key illustrating the meaning of the various colours is shown in Figure 2.4 on page 19. The run and plot commands used to generate these figures are given in the main text, and are also listed in the Appendix.

2.3.9 Stage 9 (Run): Choose `nmesh2` for Stability Calculations

Having determined the part of the δ–c plane in which periodic travelling waves exist, one can move on to a determination of their stability. The first step in this is to determine a suitable value of `nmesh2`. This constant determines the discretisation used for the periodic travelling wave solutions, and choosing a suitable value is often the most difficult part of a WAVETRAIN study. The results of previous stages show that the value `nmesh2=50`, which was inherited from the `template` directory, is large enough for the calculation of periodic travelling waves. But for studying wave stability, the discretisation using `nmesh2` is used to formulate an approximate matrix eigenvalue problem for the eigenfunctions that are periodic over one period of the wave (see §2.1.2). In many cases, it is necessary to increase `nmesh2` in order that these matrix eigenvalues and eigenvectors are a sufficiently good approximation to the actual eigenvalues and eigenfunctions.

To investigate this, one uses the command `eigenvalue_convergence`, which was discussed in §2.1.2. It is necessary to choose a few pairs of control parameter and wave speed values at which to run this command; the four pairs $(\delta, c) = (1.5, 2.0)$, $(-1.0, 2.0)$, $(-1.5, 0.1)$, $(-1.5, 3.0)$ are sensible choices. A selection of values of `nmesh2` must also be

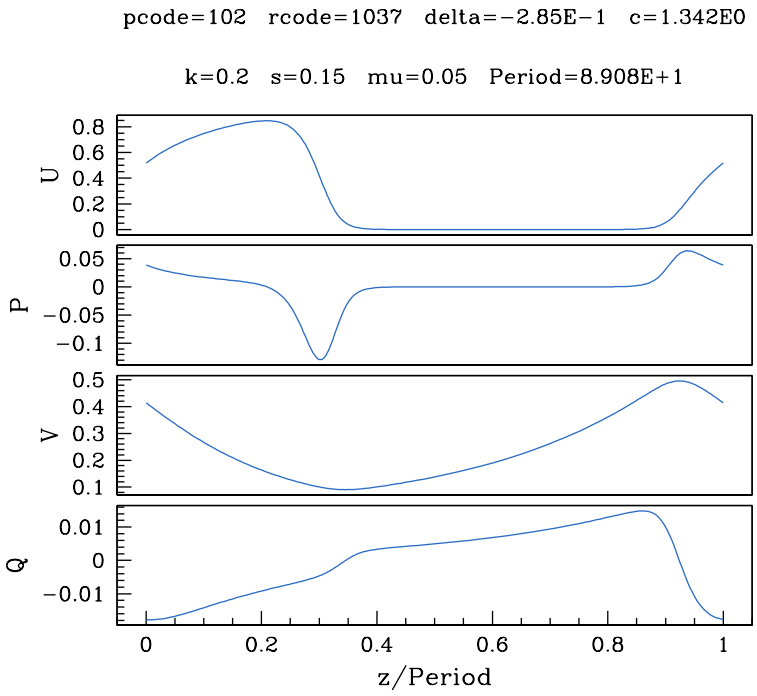


Figure 2.14: An example of a periodic travelling wave solution for the problem `workedex`. The run and plot commands used to generate this figure are given in the main text, and are also listed in the Appendix.

chosen. For most problems suitable choices would be the three values 50, 100, 200 or the four values 50, 100, 200, 400. Using the second of these for a more complete study, one runs the four commands

```
eigenvalue_convergence workedex   1.5 2.0  50 100 200 400
eigenvalue_convergence workedex  -1.0 2.0  50 100 200 400
eigenvalue_convergence workedex  -1.5 0.1  50 100 200 400
eigenvalue_convergence workedex  -1.5 3.0  50 100 200 400
```

each of which takes about 30 minutes on a typical desktop computer. The results of each of these runs should be examined for each of the 8 eigenvalues under study; here 8 is the value of `nevalues`, set in `constants.input`. Figure 2.15a shows the results for fourth eigenvalue, which are typical. Convergence is very rapid as `nmesh2` is increased for $(\delta, c) = (1.5, 2.0)$ and $(-1.5, 0.1)$. For $(\delta, c) = (-1.0, 2.0)$ convergence is slower but `nmesh2`=200 appears to give a good approximation to the eigenvalue. However for $(\delta, c) = (-1.5, 3.0)$ there is no obvious convergence pattern. To investigate this further, one can add the calculations for `nmesh2`=800, for this parameter pair only, via the command

```
eigenvalue_convergence workedex-1.5 3.0 800
```

(a)

$\delta = 1.5$, $c = 2.0$

nmesh	Re of evalue 4	Im of evalue 4	Error bound 4
50	-0.38794808E-01	0.36312786E+00	0.11995450E-12
100	-0.38928876E-01	0.36369116E+00	0.49653528E-12
200	-0.38962520E-01	0.36383359E+00	0.20041221E-11
400	-0.38971090E-01	0.36387089E+00	0.80468395E-11

$\delta = -1.0$, $c = 2.0$

nmesh	Re of evalue 4	Im of evalue 4	Error bound 4
50	0.10404277E+00	0.18641958E+00	0.46635140E-09
100	-0.26550389E-02	0.14226996E+00	0.39632024E-08
200	-0.89938986E-02	0.21837055E+00	0.17400515E-07
400	-0.90764280E-02	0.21810084E+00	0.70767272E-07

$\delta = -1.5$, $c = 0.1$

nmesh	Re of evalue 4	Im of evalue 4	Error bound 4
50	0.28543135E-01	0.70237573E-01	0.26369839E-12
100	0.28393371E-01	0.70401889E-01	0.10730430E-11
200	0.28356557E-01	0.70442488E-01	0.42990790E-11
400	0.28347372E-01	0.70452625E-01	0.17200412E-10

$\delta = -1.5$, $c = 3.0$

nmesh	Re of evalue 4	Im of evalue 4	Error bound 4
50	0.29021216E+00	0.47746546E+00	0.23805573E-09
100	0.17510311E+00	0.18398707E+01	0.16541475E-09
200	0.31235899E-01	0.22950429E+01	0.89481154E-08
400	-0.78209654E-02	0.21269384E+00	0.19689624E-06

(b)

$\delta = -1.5$, $c = 3.0$

nmesh	Re of evalue 4	Im of evalue 4	Error bound 4
800	-0.78641212E-02	0.21268068E+00	0.79270306E-06

Figure 2.15: The change in the eigenvalues of the discretised eigenfunction equations as the constant `nmesh2` is varied, with the constant `order` = 1. These two constants are defined in `constants.input`. For (a), the run commands for the four tables are listed in §2.3.9. Assuming that these are the first runs of the `eigenvalue_convergence` command for `workedex`, they will be allocated ecode values of 101–104. The tables shown can then be generated via the commands `convergence_table workedex 101 4`, `convergence_table workedex 102 4`, `convergence_table workedex 103 4`, `convergence_table workedex 104 4`. For (b), the run command is `eigenvalue_convergence workedex -1.5 3.0 800`. Assumming that the runs for (a) have been done previously, this run will be allocated an ecode value of 105. The table shown can then be generated via the command `convergence_table workedex 105 4`.

(run time about 2.5 hours on a typical desktop computer). The results for the fourth eigenvalue, which are again typical, are show in figure 2.15(b); they confirm that the eigenvalues are indeed converging, but much more slowly than for the other control parameter – wave speed pairs considered.

2.3.10 Stage 10 (Input): Change `order` in `constants.input`

The command "`set_worked_example_inputs 10`" *performs the steps described in the previous input stages of the study, and then performs the steps described in this stage.*

The results discussed in Stage 9 suggest that the value `nmesh2=400` would be suitable for an investigation of wave stability, and one could proceed on this basis. However, such a large value of `nmesh2` will lead to rather long run times, and it is therefore worthwhile investigating whether a smaller `nmesh2` is possible with a larger value of `order`. This constant is set in `constants.input`, and determines the order of the finite difference approximation used when discretising derivatives in the partial differential equations. WAVETRAIN calculates these finite difference approximations using the algorithm of Fornberg (1998). For (2.1), `order` = 1 results in a three-point approximation to the second derivatives, while `order` = 2 results in a five-point approximation. Line 12 of `constants.input` should now be changed to:

```
2 # order:  accuracy order of approx of highest spatial derivative
```

2.3.11 Stage 11 (Run): Further Tests of Eigenvalue Convergence

Having reset `order`, it is necessary to repeat the runs of `eigenvalue_convergence` for the four selected pairs of control parameter and wave speed values:

```
eigenvalue_convergence workedex   1.5 2.0  50 100 200 400
eigenvalue_convergence workedex  -1.0 2.0  50 100 200 400
eigenvalue_convergence workedex  -1.5 0.1  50 100 200 400
eigenvalue_convergence workedex  -1.5 3.0  50 100 200 400
```

each of which again takes about 30 minutes on a typical desktop computer. Figure 2.16 shows the results for fourth eigenvalue, and again the other eigenvalues show a similar convergence pattern. Comparing these results with those in Figure 2.15a shows that the convergence is significantly enhanced by the increase in `order`, enabling a smaller value of `nmesh2` to be used and hence reducing run times.

2.3.12 Stage 12 (Input): Change `nmesh1` and `nmesh2` in `constants.input`

The command "`set_worked_example_inputs 12`" *performs the steps described in the previous input stages of the study, and then performs the steps described in this stage.*

On the basis of the results described in §2.3.11, the value of `nmesh2` can now be set to 200, and `nmesh1` must also be increased to the same value. Both of these constants are set in `constants.input`.

$\delta = 1.5$, $c = 2.0$

nmesh	Re of evalue 4	Im of evalue 4	Error bound 4
50	-0.38973463E-01	0.36388020E+00	0.15821478E-12
100	-0.38973949E-01	0.36388320E+00	0.65850704E-12
200	-0.38973974E-01	0.36388341E+00	0.26704991E-11
400	-0.38973975E-01	0.36388342E+00	0.10726299E-10

$\delta = -1.0$, $c = 2.0$

nmesh	Re of evalue 4	Im of evalue 4	Error bound 4
50	0.83815416E-02	0.77199559E-01	0.11050375E-07
100	-0.91745449E-02	0.21793877E+00	0.52491508E-08
200	-0.91192530E-02	0.21801502E+00	0.23119089E-07
400	-0.91154355E-02	0.21801977E+00	0.94279284E-07

$\delta = -1.5$, $c = 0.1$

nmesh	Re of evalue 4	Im of evalue 4	Error bound 4
50	0.28345145E-01	0.70455251E-01	0.34973635E-12
100	0.28344364E-01	0.70455958E-01	0.14289575E-11
200	0.28344317E-01	0.70456000E-01	0.57298591E-11
400	0.28344314E-01	0.70456003E-01	0.22932161E-10

$\delta = -1.5$, $c = 3.0$

nmesh	Re of evalue 4	Im of evalue 4	Error bound 4
50	0.14335253E+00	0.54681288E+00	0.40620272E-07
100	0.79166525E-02	0.10178125E+01	0.12918993E-05
200	-0.78877344E-02	0.21267231E+00	0.66805176E-07
400	-0.78808884E-02	0.21267797E+00	0.26276368E-06

Figure 2.16: The change in the eigenvalues of the discretised eigenfunction equations as the constant `nmesh2` is varied, with the constant `order` = 2. These two constants are defined in `constants.input`. The run commands for the four tables are listed in §2.3.11. Assuming that the runs for Figure 2.15 have been done previously, these new runs will be allocated ecode values of 106–109. The tables shown can then be generated via the commands `convergence_table workedex 106 4`, `convergence_table workedex 107 4`, `convergence_table workedex 108 4`, `convergence_table workedex 109 4`.

2.3.13 Stage 13 (Run): Test Runs of the `stability` Command

Having chosen a value of `nmesh2`, one can move on to do some test studies of wave stability. For this, it is convenient to use the same four test pairs of δ and c as in Stages 9 and 11. Therefore one begins by running the four commands

```
stability workedex 1.5 2.0
stability workedex -1.0 2.0
stability workedex -1.5 0.1
stability workedex -1.5 3.0
```

which take only a few minutes each to run on a typical desktop computer. The first and third of these commands run successfully. However the second and fourth have numerical convergence failures, which are associated with the transition from the matrix eigenvalues and eigenvectors to the functional eigenvalues and eigenfunctions. Such convergence failures are often caused by the value of `nmesh2` being too small. However in this case the results obtained in Stage 11 give a reasonable level of confidence in the suitability of `nmesh2`, and thus the likely cause is that the value of `nmesh3` is too small.

2.3.14 Stage 14 (Input): Change `nmesh3` in `constants.input`

The command "`set_worked_example_inputs 14`" *performs the steps described in the previous input stages of the study, and then performs the steps described in this stage.*

The value of `nmesh3` must now be increased. This constant is set in `constants.input`. Its current value of 50 is inherited from the `template` input subdirectory, and 100 seems a sensible choice as a larger value.

2.3.15 Stage 15 (Run): Further Test Runs of `stability`, and a Run of `stability_loop`

The test runs of the `stability` command done in Stage 13 should now be repeated with the larger value of `nmesh3`; they all run successfully. Therefore one can move on to a loop over the δ–c plane, investigating wave stability. One does this via the command

```
stability_loop workedex
```

(run time: about 4 hours on a typical desktop computer) which loops over all 64 values in the parameter grid that is specified in `parameter_range.input`. This command runs more or less successfully, but reports 3 convergence failures. As explained in the screen output, details of these convergence failures are given in the file `combined_failures.list` in the directory `output_files/workedex/pcode103/`. Examination of this file shows that all 3 convergence failures occurred for $\delta = -2$, $c = 3$, which has an rcode value of 1008: evidently this corner of the parameter plane is a particularly difficult case. Specifically, for these parameter values WAVETRAIN has been unable to make the transition from the matrix eigenvalues and eigenvectors to the functional eigenvalues and eigenfunctions, for the first, fifth and sixth eigenvalues (ordered by the size of their real part).

Valuable insight into these convergence failures can be obtained by plotting the eigenvalue spectrum that has been calculated by WAVETRAIN in this case. One starts the plotter by typing

```
plot workedex 103
```

(103 is the pcode value for the run of `stability_loop`) and then types

```
@spectrum 1008
```

at the plotting prompt. Selecting the default axes limits gives the plot shown in Figure 2.17a. Note the open circles, which indicate the matrix eigenvalues for which there has been a convergence failure. One can focus in on the computed spectrum by rerunning

```
@spectrum 1008
```

and entering

```
-0.036 0.002 -0.05 0.4
```

as the axes limits, giving the plot shown in Figure 2.17b. There is no obvious problem with the computed spectrum, and these figures suggest that the 3 matrix eigenvalues giving convergence failures are artefacts of the discretisation. The plotter can now be exitted by typing `@exit` or `@quit`.

2.3.16 Stage 16 (Input): Change `nmesh1` and `nmesh2` in `constants.input`

The command "`set_worked_example_inputs 16`" *performs the steps described in the previous input stages of the study, and then performs the steps described in this stage.*

To confirm that the convergence failures for $\delta = -2$, $c = 3$ arise from eigenvalues that are artefacts of the discretisation, one must redo the stability calculation, for these parameters only, with a larger value of `nmesh2`. A sensible choice is to double `nmesh2`, to 400.

2.3.17 Stage 17 (Run): Run of `stability` for $\delta = -2$, $c = 3$

With the larger value of `nmesh2`, one should now run the command

```
stability workedex -2.0 3.0
```

(run time: about 30 minutes on a typical desktop computer). The number of previous runs of either `ptw` or `stability` will depend on the number of tests that have been run in previous stages, and this will affect the rcode value allocated to this new run, but 1022 would be a typical rcode value. The run is successful, with no convergence failures. To view the computed spectrum, one starts the plotter via

```
plot workedex
```

and then enters the command

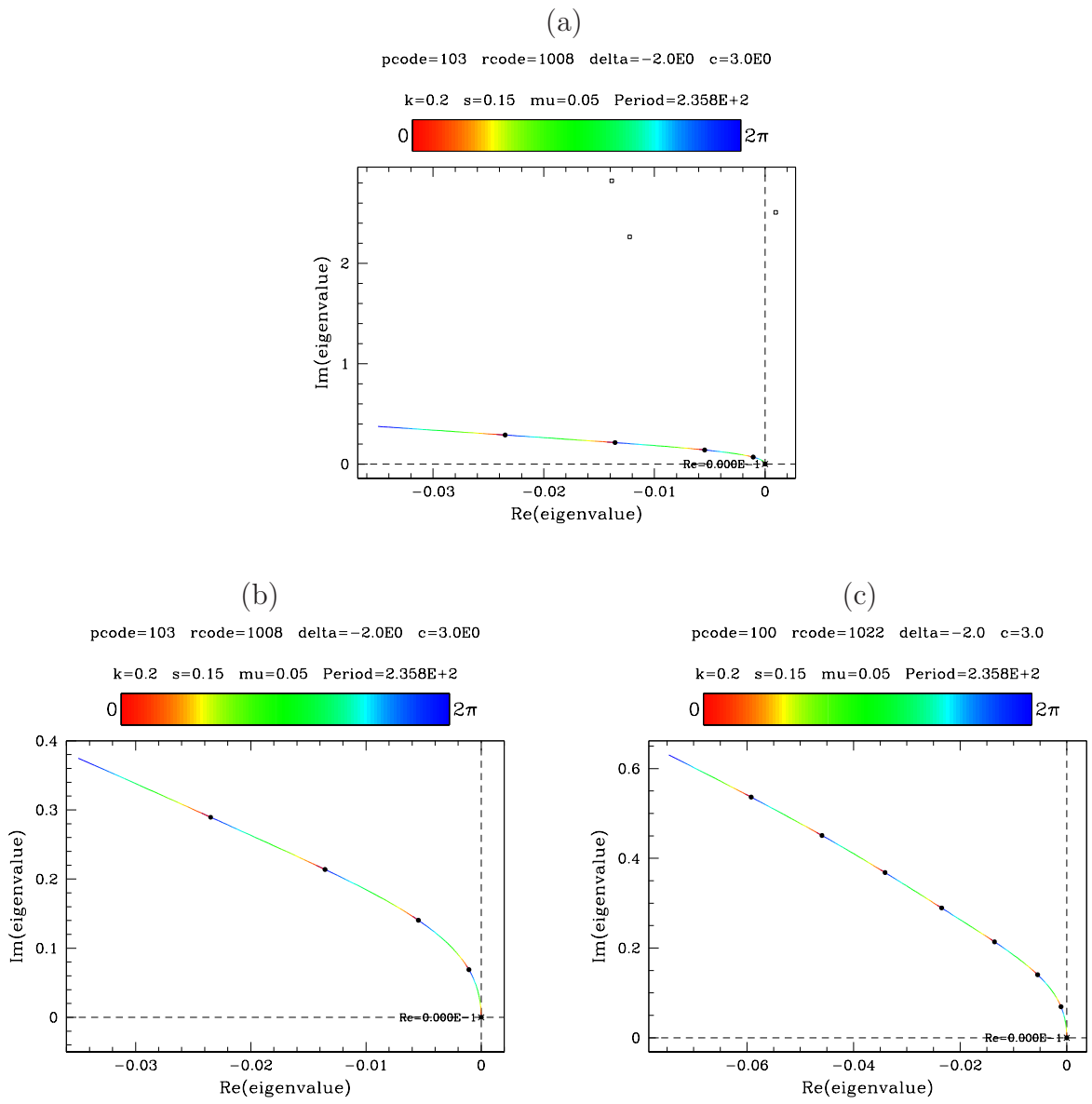


Figure 2.17: Plots of the calculated eigenvalue spectrum for $\delta = -2$, $c = 3$. (a) The plot given by the `@spectrum` command with default axes limits. The open circles denote matrix eigenvalues that gave numerical convergence failure when used as a starting point for calculating the spectrum; the closed circles denote matrix eigenvalues from which spectrum continuation was successful. The value of `nmesh2` was 200 in this case. (b) The same results as (a), but with manually input axes limits. (c) The calculated spectrum with `nmesh2`=400. The are no numerical convergence failures in this case, and default axes limits were used in the plot. The run and plot commands used to generate these figures are given in the main text, and are also listed in the Appendix. Note that if plotting is done using `gnuplot` then ticmarks will be absent from the horizontal axis in these plots; this applies if `spectrumcolour` is set to `rainbow` or `greyscale` or `grayscale`, but not if a single colour is used.

```
@spectrum 1022
```

selecting the default axis limits; the resulting plot is shown in Figure 2.17c. It has the same appearance as the spectrum calculated with `nmesh2`=200 and shown in Figure 2.17b, except that it extends to more negative values of the real part of the eigenvalue; this is because three additional "genuine" eigenvalues have replaced those that were artefacts of the discretisation. The plotter can now be exitted by typing `@exit` or `@quit`.

When some of the matrix eigenvalues give convergence failures, WAVETRAIN assesses the wave as stable or unstable based on the part of the eigenvalue spectrum that was calculated using the other matrix eigenvalues. Thus when WAVETRAIN studied the case $\delta = -2$, $c = 3$ as part of the parameter loop in Stage 15, it assessed the wave as being stable. The calculations in this section confirm that this assessment was correct.

2.3.18 Stage 18 (Input): Reset `nmesh1` and `nmesh2` in `constants.input`

The command "`set_worked_example_inputs 18`" *performs the steps described in the previous input stages of the study, and then performs the steps described in this stage.*

Before proceeding, it is necessary to reset `nmesh1` and `nmesh2` to 200.

2.3.19 Stage 19 (Run): Plot the Results of the `stability_loop` Run

Having clarified the situation for $\delta = -2$, $c = 3$, one can proceed with plotting the results of the `stability_loop` run done in Stage 15. One starts the plotter by typing

```
plot workedex 103
```

(103 is the relevant pcode value) and then types

```
@pplane
```

at the plotting prompt. Selecting the default plot type (rcode numbers) gives the plot shown in Figure 2.18. There are two separate parameter regions giving stable waves, separated by a region in which waves are unstable.

2.3.20 Stage 20 (Run): Run of `stability_boundary`

The next stage of the study is to trace the boundaries in the δ–c plane between the regions of stable and unstable periodic travelling waves. It is clear from Figure 2.18 that there are two such boundaries. The starting point for calculating them are pairs of points in the δ–c plane lying on either side. For the right hand boundary, suitable points correspond to rcodes 1019 and 1020, which correspond to $c = 2.171$ with $\delta = 0.857$ and $\delta = 0.285$ respectively. Therefore one types

```
stability_boundary workedex 103 0.857 2.171 0.285 2.171
```

(run time: about 15 minutes on a typical desktop computer). For the left hand boundary, rcode values 1022 and 1023 lie either side; these have $c = 2.171$ with $\delta = -0.857$ and $\delta = -1.428$ respectively. Therefore one types

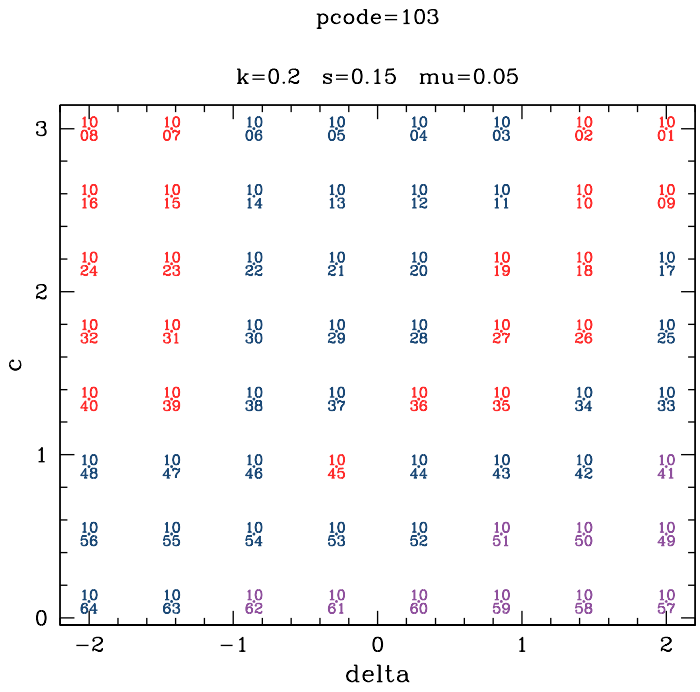


Figure 2.18: Results on the stability of periodic travelling wave solutions for the problem `workedex`. A key illustrating the meaning of the various colours is shown in Figure 2.4 on page 19. The run and plot commands used to generate these figures are given in the main text, and are also listed in the Appendix.

```
stability_boundary workedex 103 -0.857 2.171 -1.428 2.171
```

(run time: about 15 minutes on a typical desktop computer).

To visualise these stability boundaries, one must first restart the plotter via

```
plot workedex 103
```

and replot the parameter plane via

```
@pplane
```

entering `symbol` as the plot type for variety. One then adds the stability boundaries via the command

```
@stability_boundary all
```

giving the plot shown in Figure 2.19. Although the commands have run successfully, both stability boundary curves in Figure 2.19 are rather jagged in appearance. This indicates that the continuation step sizes are somewhat too large.

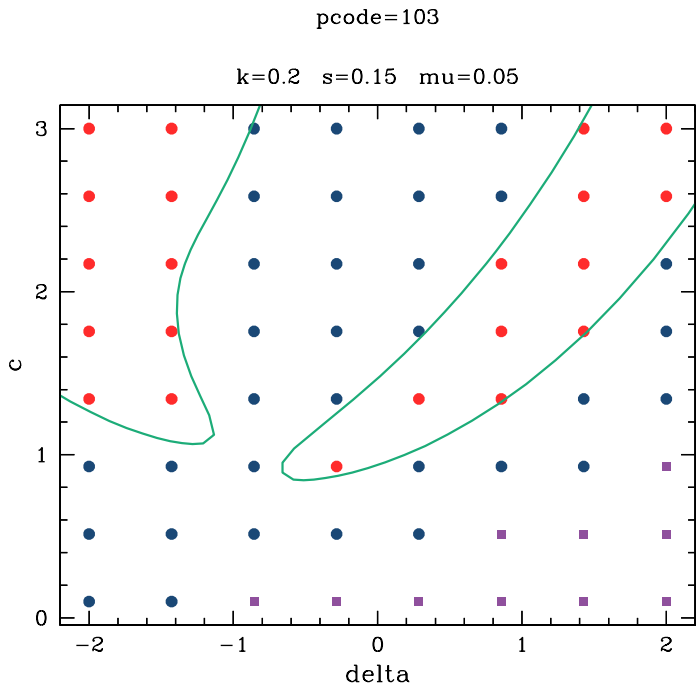


Figure 2.19: Results on the existence of periodic travelling wave solutions, including the boundaries between parameter regions giving stable and unstable waves, for the problem `workedex`. The stability boundaries are visibly jagged, due to the continuation step sizes being too large. A key illustrating the meaning of the various colours is shown in Figure 2.4 on page 19. The run and plot commands used to generate these figures are given in the main text, and are also listed in the Appendix.

2.3.21 Stage 21 (Input): Reduce the Step Sizes for `stability_boundary`

The command "`set_worked_example_inputs 21`" *performs the steps described in the previous input stages of the study, and then performs the steps described in this stage.*

A factor of 10 should be ample as a reduction in the step size settings for stability boundary calculations. Therefore line 9 of `constants.input` should be changed to:

```
0.01 0.005 0.05 # ds(>0),dsmin,dsmax for stability boundary calcs
```

2.3.22 Stage 22 (Run): Rerun of `stability_boundary`

The two commands

```
stability_boundary workedex 103 0.857 2.171 0.285 2.171
stability_boundary workedex 103 -0.857 2.171 -1.428 2.171
```

should now be rerun. The run time for each is about 30 minutes on a typical desktop computer. Plotting these new stability boundaries (see Figure 2.21 below) confirms that

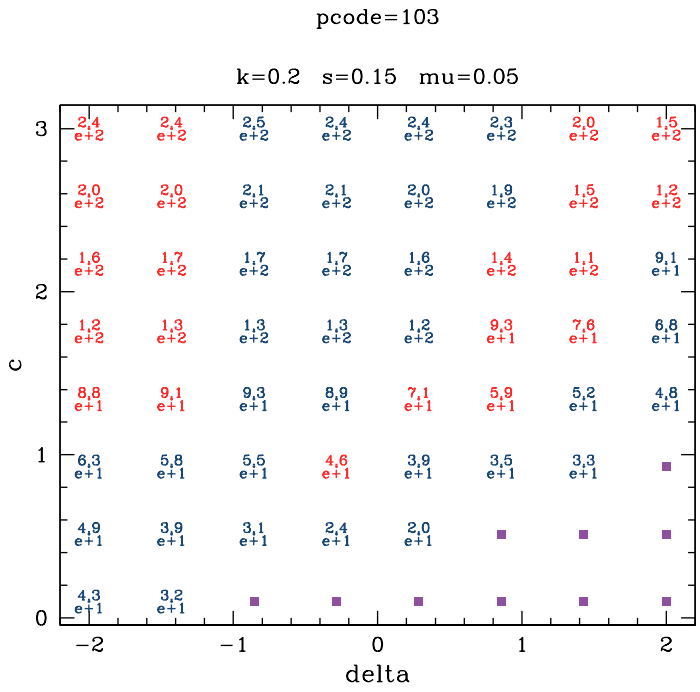


Figure 2.20: Results on the stability of periodic travelling wave solutions for the problem `workedex`, with results displayed using the period of the waves. A key illustrating the meaning of the various colours is shown in Figure 2.4 on page 19. The run and plot commands used to generate these figures are given in the main text, and are also listed in the Appendix.

they have a smooth appearance.

2.3.23 Stage 23 (Run): Calculate Contours of Constant Period

There is no need to calculate contours of constant period, but it can be helpful in understanding the periodic travelling wave family. To determine suitable contour levels, it is helpful to replot the δ–c plane, showing wave periods rather than rcode values or symbols. To do this one types

```
@pplane
```

at the plotter prompt, entering `period` for the plot type. The resulting plot is now shown in Figure 2.20. This shows that 50, 100, 150 and 200 are suitable contour levels. In each case, the `period_contour` command requires two points in the δ–c plane lying either side of the contour, and these can easily be read off Figure 2.20. Having exitted the plotter via `@exit` or `@quit`, one can then run the commands to calculate the period contours, with suitable commands being

```
period_contour workedex 103 period=50 -1.0 0.9 -0.2 0.9
period_contour workedex 103 period=100 0.85 1.6 0.85 2.2
period_contour workedex 103 period=150 0.9 2.2 0.2 2.2
period_contour workedex 103 period=200 1.0 2.6 -0.4 2.6
```

which calculate the various contours.

2.3.24 Stage 24 (Input): Copy PDE Simulation Data File

The command "`set_worked_example_inputs 24`" *performs the steps described in the previous input stages of the study, and then performs the steps described in this stage.*

Before plotting the results of the period contour calculations, it is instructive to add one further ingredient to the plot. Smith & Sherratt (2007) present results from numerical simulations of the partial differential equations (2.1) on a large domain with zero Dirichlet boundary conditions, for a range of values of δ, with $k = 0.2$, $s = 0.15$ and $\mu = 0.05$ as in this worked example. In each case periodic travelling waves develop. Their results are reproduced in the files `documentation/worked_example/stage24/pde_stable.data` and `documentation/worked_example/stage24/pde_unstable.data`. These files contain two columns, which are the δ values and the measured values of the wave speed, with the two files corresponding to values of δ for which there was not or was visible evidence of instability in the waves. The data in these files can be incorporated into WAVETRAIN plots via the plot command `@pointsfile` (see page 116), and the files should now be copied into the `workedex` input subdirectory.

2.3.25 Stage 25 (Run): Final Plots

The various results can now be gathered together in a final plot. Firstly, in order to include the locus of Hopf bifurcation points in this plot it is necessary to recalculate it for pcode 103, via the command

```
hopf_locus workedex 103 1 0 1 6
```

(alternatively one could use the `copy_hopf_loci` command, although WAVETRAIN would issue queries because of the differences in the input files between pcode 103 and pcodes 101/102). One then starts the plotter via

```
plot workedex 103
```

and enters the plotter command

```
@pplane
```

entering `symbol` as the plot type, which is most suitable for a final plot. One then enters the commands

```
@hopf_locus 101
@stability_boundary 103
@stability_boundary 104
```

to add the locus of Hopf bifurcation points and the stability boundaries. Note that 103 and 104 are the scode values for the runs of `stability_boundary` done in Stage 22, with reduced step sizes. To add the period contours, one enters

```
@period_contour all
```

at the plotter prompt. The user is then prompted about the location of contour labels. By default these are placed at the edges of the plot, but in this case a clearer plot is given by entering

```
delta=-1.8 delta=1.55
```

as the label location. Finally the data from the partial differential equation simulations is added to the plot via the two commands

```
@pointsfile pde_stable.data 9
@pointsfile pde_unstable.data 8
```

where the second arguments (`9` and `8`) specify that closed and open triangles are to be used for the two data sets; a full list of WAVETRAIN symbol codes is given on page 127. The resulting plot is shown in Figure 2.21. Note that one of the data points from the partial differential equation simulations lies in the unstable region of the parameter plane, but has been recorded as stable. This is entirely expected: the space and time scales over which the instabilities develop is too long for them to be manifested visibly in the simulations. The plotter should now be exitted via `@exit` or `@quit`.

The plot shown in Figure 2.21 gives a full account of the results, but visually it is rather busy. The user may prefer a picture without the coloured dots and squares indicating the (δ, c) points used in the `stability_loop` run. To generate this it is necessary to create a blank parameter plane using the command

```
new_pcode workedex
```

which assigns pcode value 104 to the new parameter plane. One then copies the various results across via the commands

```
copy_hopf_loci 103 104
copy_period_contours 103 104
copy_stability_boundaries 103 104
```

and types

```
plot workedex 104
```

to restart the plotter. One then simply repeats the series of plotter commands used to generate Figure 2.21; the only difference is that the `@pplane` command does not prompt the user for the plot type, since no (δ, c) points are being plotted. The resulting plot is shown in Figure 2.22.

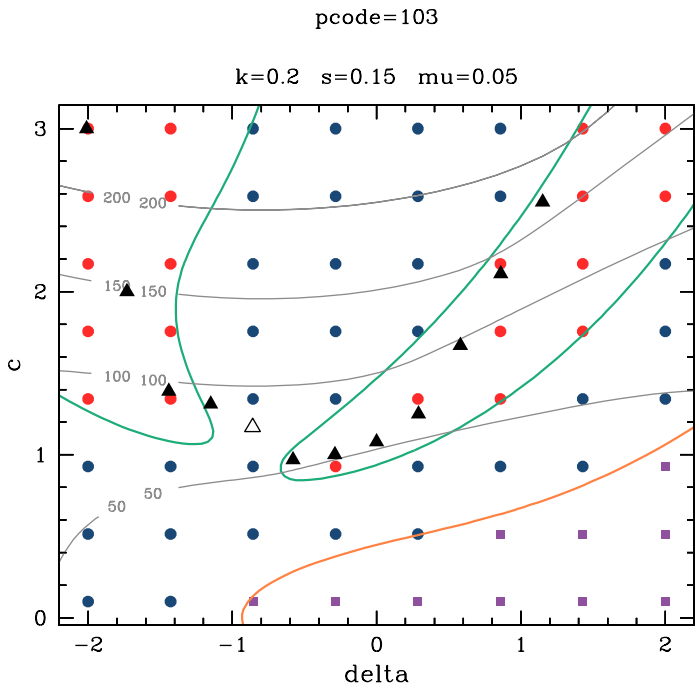


Figure 2.21: A final plot of the control parameter–wave speed plane for the problem `workedex`. A key illustrating the meaning of the various colours and symbols is shown in Figure 2.4 on page 19, except for the black triangles, which indicate results from numerical simulations of the partial differential equations. Open/closed triangles indicate solutions with/without visible evidence of instability (see main text for details). The run and plot commands used to generate these figures are given in the main text, and are also listed in the Appendix.

2.3.26 Stage 26 (Run): Delete Unwanted Output Files

WAVETRAIN generates significant amounts of numerical data. To avoid this accummulating, it is good practice to remove unwanted output files at the end of a study. A series of commands are provided for this purpose, and they are described in detail in §3.1.6. For this worked example, all runs associated with pcode values 101 and 102 are now redundant, and the corresponding output files can be deleted via the commands

```
rmpcode workedex 101
rmpcode workedex 102
```

which prompt the user for confirmation. In addition, the data files associated with the large number of runs of `ptw`, `stability` and `eigenvalue_convergence` are all no longer needed. All WAVETRAIN runs such as these, which are not associated with a parameter plane plot, have their output data stored under the notional pcode value 100 (see §3.1.6 and §4.4 for further details). Therefore the output data can be deleted via the command

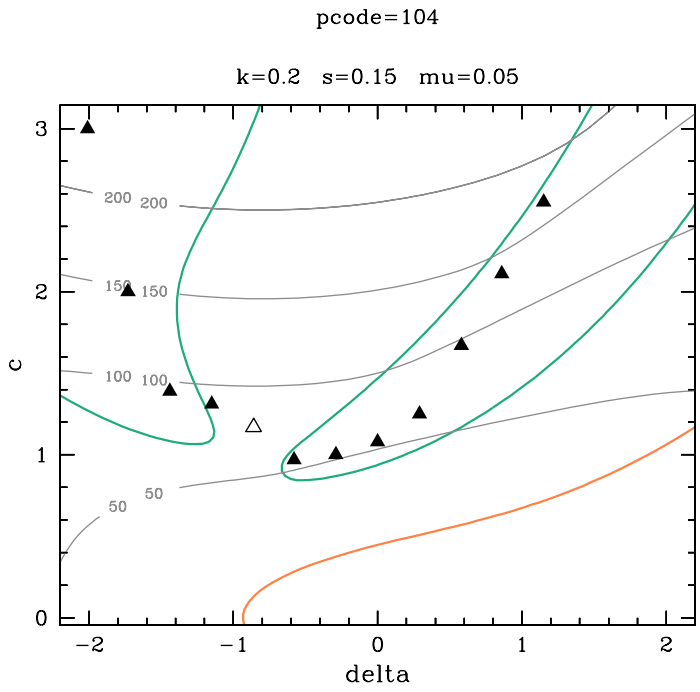


Figure 2.22: An alternative version of the final plot of the control parameter–wave speed plane for the problem `workedex`. This figure is the same as Figure 2.21 except that the symbols indicating the (δ,c) points used in the run of `stability_loop` are omitted. A key illustrating the meaning of the various colours and symbols is shown in Figure 2.4 on page 19, except for the black triangles, which indicate results from numerical simulations of the partial differential equations. Open/closed triangles indicate solutions with/without visible evidence of instability (see main text for details). The run and plot commands used to generate these figures are given in the main text, and are also listed in the Appendix.

```
rmpcode workedex 100
```

which issues three separate prompts for confirmation, since this command has the potential to delete a large amount of output data.

2.4 Documentation and Help Facilities

In the main WAVETRAIN directory there is a subdirectory `documentation` containing a PDF copy of this user guide.

A basic help facility is provided in WAVETRAIN via the command `wt_help`; like all commands, the user must be in the main WAVETRAIN directory to use it. Typing

```
wt_help <command>
```

provides a brief summary of the usage of the specified command, which can be either a run or plot command. If no argument is given, `wt_help` lists the WAVETRAIN run and plot commands. By default the output from `wt_help` is scrolled on the screen, but this can be changed to a listing of the appropriate help file by editting `defaults.input`.

Help for plotter commands is also available from within the plotter. Typing `@help` followed by a command name gives a summary of the command's syntax and usage. Typing `@help` alone gives a listing of the plot commands. By default the plot command `@help` scrolls through the corresponding help file, but this can be changed to a listing by changing `helpdisplay` in `plot_defaults.input`.

For the benefit of users wishing to understand the workings of WAVETRAIN, each subdirectory contains a `README` file that summarises the role played by each program within it. There is also a `README` file in the main WAVETRAIN directory, which contains the version name/number.

2.5 Troubleshooting

It is anticipated that most users will run WAVETRAIN commands interactively, with the constant `info` set to 3 (in `constants.input`). This results in limited screen output, charting the overall progress of the run. If a problem occurs, then this screen output may be sufficient to resolve it. Otherwise, or if `info` is set to 1 or 2, users can see much more detailed information on the run in a file called `info.txt`. This file will be located in a subdirectory of `output_files`. Full details of the subdirectory structure of `output_files` are given in §4.4.1, and the following list simply gives the location of `info.txt` files associated with the various WAVETRAIN commands.

`bifurcation_diagram` This command has not yet been discussed: see §3.1.5. Detailed information on a run of this command is contained in
`output_files/pcode100/bcode<code_number>/info.txt`

`eigenvalue_convergence` Detailed information on a run of this command is contained in `output_files/pcode100/ecode<code_number>/info.txt`

`hopf_locus` Detailed information on a run of this command is contained in
`output_files/pcode<code_number>/ccode<code_number>/info.txt`

`period_contour` Detailed information on a run of this command is contained in
`output_files/pcode<code_number>/ccode<code_number>/info.txt`

`ptw` and `stability` Detailed information on a run of these commands is contained in
`output_files/pcode100/rcode<code_number>/info.txt`

`ptw_loop` and `stability_loop` Detailed information on a run of these commands is divided between a number of different `info.txt` files. Details of overall progress through the loop over the grid of control parameter and wave speed values is contained in `output_files/pcode<code_number>/info.txt` and specific information about the run for a given pair of control parameter and wave speed values is contained in `output_files/pcode<code_number>/rcode<code_number>/info.txt`

`stability_boundary` Detailed information on a run of this command is contained in `output_files/pcode<code_number>/scode<code_number>/info.txt`

One component of these `info.txt` files is a list of any errors and warnings that have occurred during the run. For convenience, this list is reproduced in a file `errors.txt` in the same subdirectory. (If no errors or warnings have occurred, this file will be present but empty).

During runs of its various commands, WAVETRAIN generates a large number of temporary files (see §4.3.1 for details). By default, these files are deleted at the end of a run, but they can be retained by setting the constant `iclean` to 2 in `constants.input`. In some cases, this can also be useful in attempting to understand the cause of a problem. Once the files have been examined, they can be deleted by the command `cleanup`.

Part 3

Advanced Features of WAVETRAIN

3.1 Further Details of Run Commands

3.1.1 The Format of Numerical Inputs, and Precision

Numerical inputs to WAVETRAIN are required in the various input files, and also as command arguments. They can be supplied in either decimal or scientific notation. Thus `123.4`, `1.234E2` and `1.234E+2` are all acceptable. Entries that happen to be integer-valued can also be entered without a decimal point: for example the control parameter value `3.0` can also be entered as `3`. However there is one important case in which an integer value and its decimal equivalent are treated differently, namely in powers that appear in `equations.input`. A term such as "`x**3`" in `equations.input` is evaluated as one would expect, by multiplying `x` by itself three times; however "`x**3.0`" is evaluated using the logarithm and exponential functions, which is less accurate. Therefore to preserve accuracy, integer powers should always be entered as integers. Of course, integer variables such as the numbers of grid points in `parameter_range.input` must be given as integers.

WAVETRAIN does its computations using Fortran77 programs, which are written by the package on the basis of the input files. It uses 8-byte ("double") precision throughout, meaning that there are 16 significant decimal digits. Users who are familiar with Fortran77 will know that this level of precision requires that numerical values are specified explicitly as being double precision. For example `1.0/3.0` gives only eight 3's after the decimal point, with the remaining digits being random; in Fortran77 one must instead write `1.0D0/3.0D0`. WAVETRAIN takes account of this when converting the input files into Fortran77 code, changing `E`'s to `D`'s in scientific notation and adding "`D0`" to decimals and "`.0D0`" to integers in order to retain double precision accuracy throughout. An important exception to this is integer powers, which are left as integers (see the discussion in the previous paragraph).

A final point about numerical format concerns upper and lower case. According to the international standard for Fortran77 (see `http://gcc.gnu.org/wiki/GFortranStandards` and `http://rsusu1.rnd.runnet.ru/develop/fortran/prof77/index.html`), programs must be written entirely in upper case, and this is true for all code used in WAVETRAIN. However, in principle, this should also apply to numerical inputs. Thus a numerical input such as `1.234e2` is not compatible with the international standard for Fortran77: it

should be `1.234E2`. In reality, all modern Fortran77 compilers will accept both lower and upper case, but it is conceivable that a user might have a Fortran77 compiler that gives an error because of entries with a lower case "`e`". In this highly unlikely event, the remedy is simple: change to upper case "`E`" in any numerical values entered using scientific notation.

3.1.2 Optional Arguments of the `stability_boundary` Command

The command `stability_boundary` has five compulsory arguments; the first is the subdirectory name, and arguments 2–5 are the coordinates of two points in the control parameter–wave speed plane lying on either side of the stability boundary. It is also permissible to give additional argument(s). These have one of two possible forms: either <control_parameter_name>=<value> or <wave_speed_name>=<value>. Here the labels "<control_parameter_name>" and "<wave_speed_name>" denote the names of the control parameter and the wave speed, as given in `variables.input`. There is no upper limit on the number of such additional arguments, and they cause detection of points at which the stability boundary crosses the specified values; if there are multiple crossings, they are all recorded. These crossings are written to the output file `info.txt`, and also to the screen if the constant `info` (defined in `constants.input`) is 3 or 4. They can be retrieved subsequently via the command `list_crossings`. Thus for the example problem `demo` discussed in the previous section, the command

```
stability_boundary demo 102 1.75 0.3 1.75 0.7 A=0.7 c=0.55 A=1.1 A=2.5 c=0.65
```

causes the stability boundary to be calculated as described in §2.1, but with the additional recording of the points at which the stability boundary crosses $A = 0.7$, 1.1, 2.5 and $c = 0.55$, 0.65. If no subsequent runs have been done other than those listed in §2.1 then this run will be allocated the scode value 102, and the command

```
list_crossings demo 102 102
```

will give a list of the crossing points. (Here the first 102 is the pcode value and the second is the scode value). The crossing information is not used in plotting.

3.1.3 The Commands `set_homoclinic` and `unset_homoclinic`

WAVETRAIN does not have the capability to track the loci of actual homoclinic solutions of the travelling wave equations. Rather, these must be approximated by the loci of solutions of large period, as discussed in §2.1. For the purposes of plotting, it is often convenient to represent such a locus differently from that of other contours of constant wave period. Typing `set_homoclinic demo 102 101` (for example) designates the contour with ccode 101 for the parameter plane with pcode 102 to be an (approximation to) a locus of homoclinic solutions. This is simply a relabelling: no new computation is done. Its effect is that the plotter command `@period_contour` plots that contour in a different colour, and omits the label(s) showing the value of the period. The designation can be reversed by typing `unset_homoclinic demo 102 101`. Note that if `set_homoclinic`/`unset_homoclinic` are

applied to a contour that is currently designated as being/not being homoclinic, it simply has no effect. (No error is reported.)

As an example of the use of these commands, consider the plot shown in Figure 2.5 on page 22. This plot was for a run with pcode 101, and shows a control parameter–wave speed plane with two contours of constant wave period, with periods 3000 (ccode 101) and 80 (ccode 102). Typing

```
set_homoclinic demo 101 101
```

designates the first of these to be a locus of homoclinic solutions. Replotting via

```
plot demo 101
```

followed by the plot command

```
@pplane
```

(selecting `symbol` as the plot type) and then

```
@hopf_locus 101
```

and

```
@period_contour all
```

(selecting the default label location) gives the plot illustrated in Figure 3.1. The contour of period 3000 is shown in a different colour and weight, and without labels showing the period.

For ease of coding, the plot command `@period_contour` prompts the user about the location of contour labels even if all of the contours being plotted have been designated as homoclinic. No use is made of the user's response in this case.

3.1.4 The Command `new_pcode`

Having calculated the parameter plane for demo, as described in §2.1, one may wish to obtain the corresponding plot for a slightly different value of one of the other parameters, for instance $B = 0.4$ rather than $B = 0.45$. (Recall that these parameters are given in the file `other_parameters.input`). One might naturally assume that the basic structure of the plot would be the same, making a scan across the parameter plane unnecessary: one would just need to recompute the locus of Hopf bifurcation points, the "homoclinic" locus, and the stability boundary. To do this one requires a pcode value, which has previously been generated via a run of `ptw_loop` or `stability_loop`. The command `new_pcode` is provided for this situation; it was introduced previously in §2.3. After editting the file `other_parameters.input`, one types

```
new_pcode demo
```

and the new pcode value is reported. The commands `hopf_locus`, `period_contour` and `stability_boundary` can then be used to generate all the data for the parameter plane plot. Note that if the plot command `@pplane` is used for a pcode value created via `new_pcode`, it causes axes, labels and titles to be drawn around a blank plot; this is necessary before using the plot commands `@hopf_locus`, `@period_contour` or `@stability_boundary`.

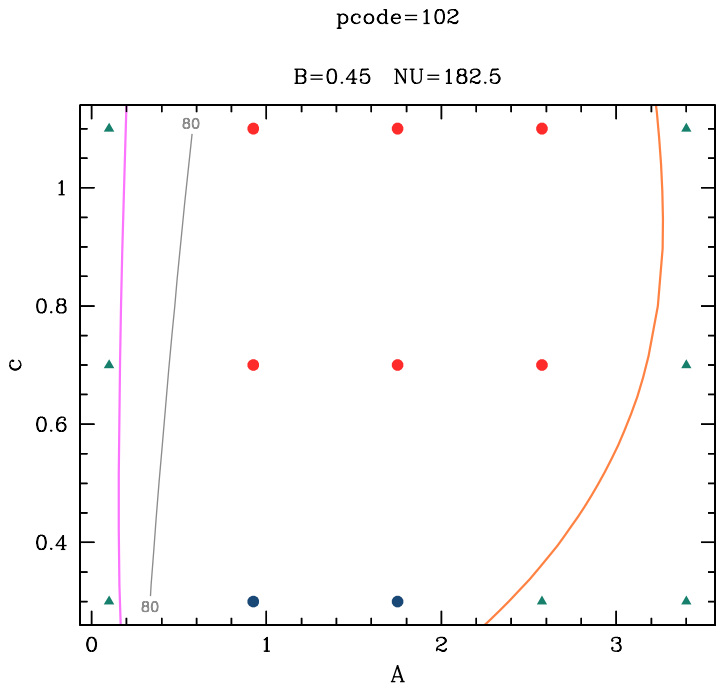


Figure 3.1: An illustration of the use of the run command `set_homoclinic`. The figure shows the Hopf bifurcation locus and two contours of constant wave period for the problem `demo`, one of which has been designated to be a locus of homoclinic solutions. These curves are superimposed on a plot showing periodic travelling wave existence in the control parameter–wave speed plane. A key showing the meaning of the various symbols and colours (including that used for the homoclinic locus) is shown in Figure 2.4 on page 19. The run and plot commands used to generate this figure are given in the main text, and are also listed in the Appendix.

3.1.5 The Command `bifurcation_diagram`

The main capability of WAVETRAIN that was not discussed in section 2.1 is the generation of bifurcation diagrams. The basic command has a form such as

```
bifurcation_diagram demo c=0.8
```

which generates a bifurcation diagram as the control parameter is varied, for wave speed `c`= 0.8. (The wave speed name `c` is set in the file `variables.input`). The limits on the control parameter for the bifurcation diagram are taken from `parameter_range.input`. The run is allocated a three digit "bcode" number (101-999); since this is the first bifurcation diagram run, the bcode will be 101. The diagram can be plotted by starting the plotter via

```
plot demo
```

(no pcode value is needed) and then running the plotter command

```
@bifurcation_diagram 101
```

(101 is the bcode value). The user is asked to specify whether the vertical axis of the plot should show the L2-norm of the travelling wave solution and/or the L2-norm of the steady state, or the wave period. There is also the opportunity to manually override the default axis limits, which is often necessary when using the wave period if the plotting region includes a homoclinic solution. Selecting "`norm`" for the vertical axis and default axis limits gives the plot shown in Figure 3.2a.

As an alternative to specifying a wave speed value and using the control parameter as the bifurcation parameter, the roles can be reversed. For example the command

```
bifurcation_diagram demo A=2.6
```

will generate a bifurcation diagram with the wave speed as the bifurcation parameter; this is illustrated in Figure 3.2b. (The control parameter name `A` is set in the file `variables.input`).

The `bifurcation_diagram` command also has an optional additional argument, which is the name of one of the travelling wave variables (as specified in `variables.input`). If this is included then the same computations are performed but with different output data. Rather than recording the L2-norm of the whole travelling wave solution, the maximum, minimum, mean, L2-norm and steady state value of the specified variable are recorded. One can select which of these are plotted when one runs the plot command `@bifurcation_diagram`. An example run command would be

```
bifurcation_diagram demo variable=W c=0.6
```

which will be allocated a bcode value of 103 since it is the third bifurcation diagram to be calculated. Here the order of the second and third arguments does not matter, so that

```
bifurcation_diagram demo c=0.6 variable=W
```

is equivalent. To plot the resulting bifurcation diagram, one starts the plotter by typing

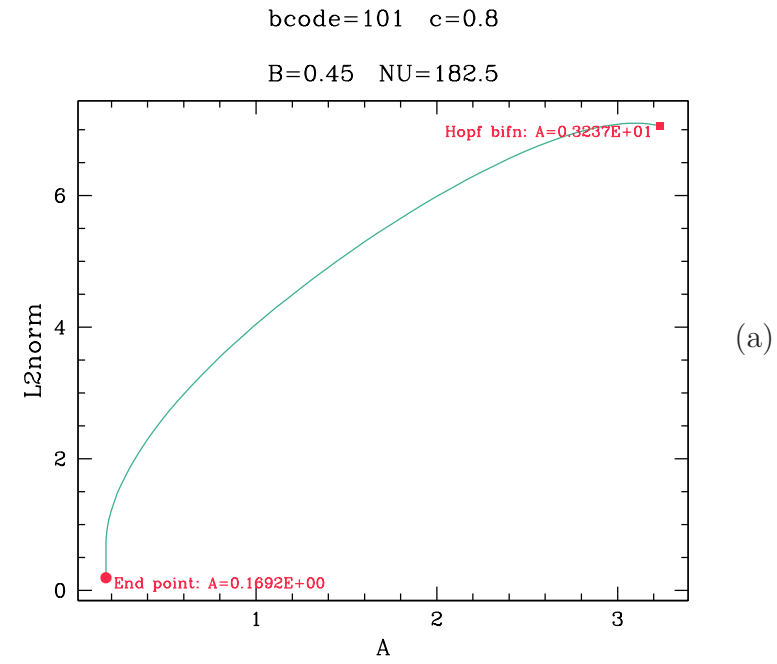
```
plot demo
```

and then gives the plot command

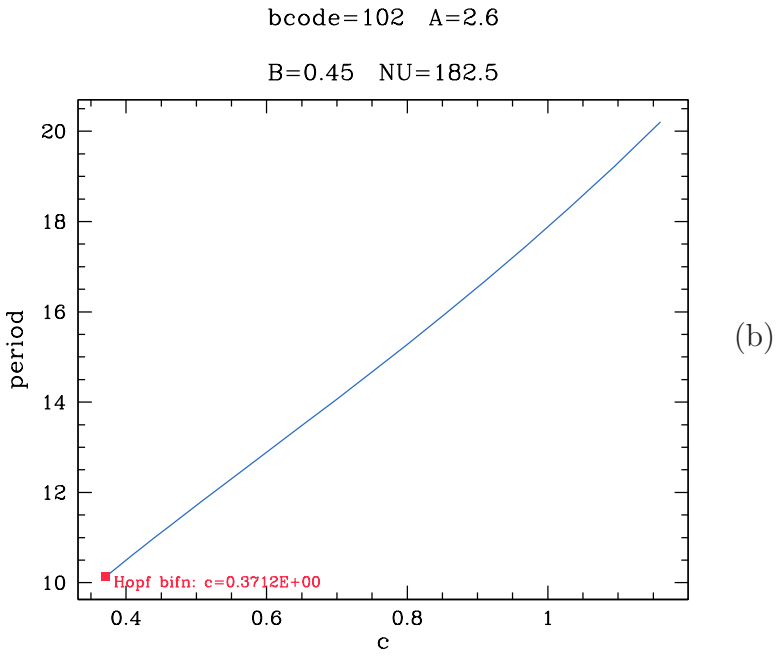
```
@bifurcation_diagram 103
```

(103 is the bcode value). The user will then be prompted to choose from a variety of different options for what is shown on the vertical axis. For example, selecting "`mean max min`" gives the plot shown in Figure 3.3a, while "`max mean stst`" gives the plot shown in Figure 3.3b. In both cases, the plots shown use the default axes limits. Note that the legend boxes are included automatically when there is more than one solution property in the plot.

A final comment concerning the `bifurcation_diagram` command is that it is necessary that there is a Hopf bifurcation within the relevant parameter range. For example, the command

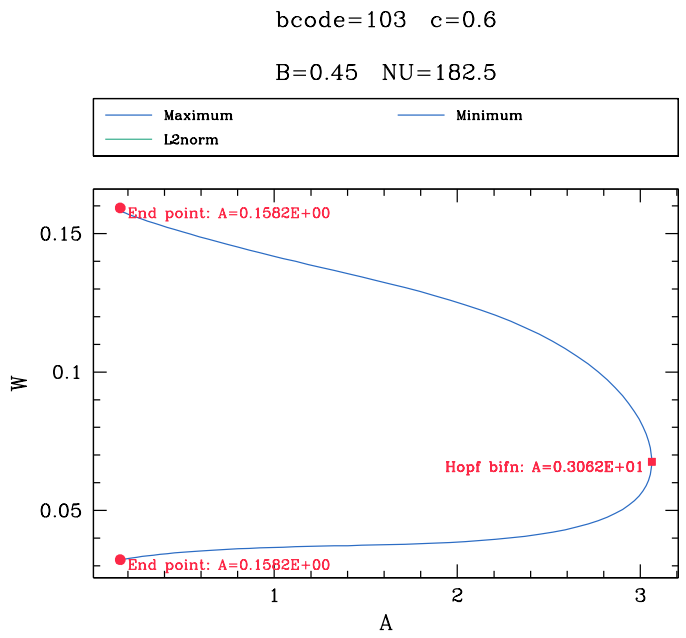


(a)

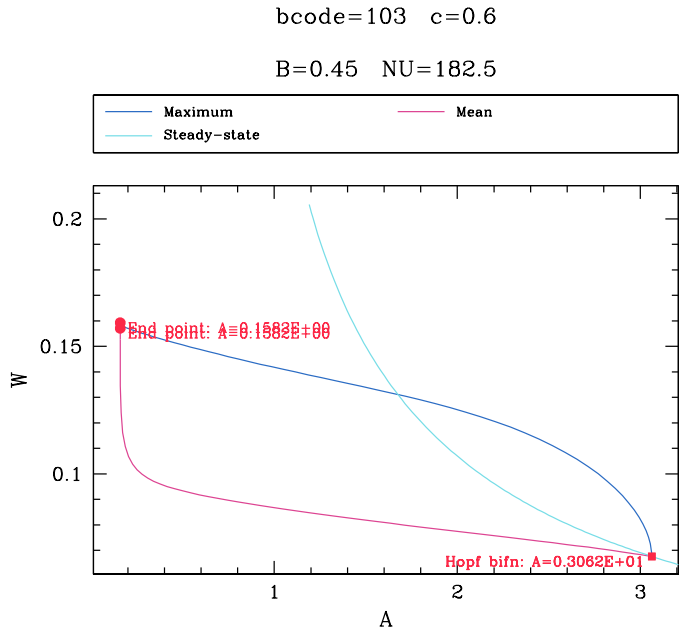


(b)

Figure 3.2: Bifurcation diagrams for the problem `demo`. The control parameter and wave speed as used as the bifurcation parameter in (a) and (b) respectively. The L2-norm of the solution is plotted on the vertical axis in (a), and the period is used in (b). The run and plot commands used to generate these figures are given in the main text, and are also listed in the Appendix.



(a)



(b)

Figure 3.3: Bifurcation diagrams for the problem `demo`, with W specified as the study variable in the command line. Parts (a) and (b) are for the same run, but with different options selected for the vertical axis. Note that the same line colour is used for the maximum and minimum; this can be changed by altering `bdlinecolourmax` and/or `bdlinecolourmin` in the plotter style file (see §3.4.2). The run and plot commands used to generate these figures are given in the main text, and are also listed in the Appendix.

```
bifurcation_diagram demo A=2.0
```

would return an error message saying that no Hopf bifurcation was found as the wave speed c varied between 0.3 and 1.1 (specified in `parameter_range.input`) for $A = 2.0$. Note that there is a periodic travelling wave solution for all wave speeds in this range, but WAVETRAIN cannot calculate the solution branch without its starting point, namely a Hopf bifurcation. Similarly

```
bifurcation_diagram demo A=0.5
```

fails to calculate a bifurcation diagram, although in this case the reason is that there is no steady state for $A = 0.5$. Of course, there may be more than one Hopf bifurcation point in the parameter range. This does not pose any difficulties for the `bifurcation_diagram` command, which will calculate the solution branch emanating from each of the Hopf bifurcation points.

3.1.6 Commands for Deleting Data Files

WAVETRAIN generates a large number of data files, in a large number of output subdirectories. Manual deletion of unwanted files and directories would be very laborious, and thus WAVETRAIN provides a series of commands for systematic deletion. The command

```
rmrcode demo 1002
```

deletes all of the data files associated with the run of `ptw` or `stability` that was allocated the rcode value 1002. For runs associated with loops through the control parameter–wave speed plane (via the `ptw_loop` or `stability_loop` commands), the pcode value must also be specified; thus

```
rmrcode demo 101 1002
```

deletes the run with rcode 1002 for pcode 101. Note that in all WAVETRAIN commands, if a pcode value is needed as an argument, it is always given as the second argument, following the subdirectory name. One final point concerning the command `rmrcode` is that for the purposes of file classification (see §4.4.1), all runs of `ptw` and `spectrum` are allocated to the dummy pcode value of 100. Thus the commands

```
rmrcode demo 102
```

and

```
rmrcode demo 100 102
```

are equivalent.

Sometimes one may wish to delete files associated with all rcode values, for a particular pcode. To achieve this, one replaces the rcode number by `all` in the above commands. (`All` or `ALL` are also allowed).

The commands `rmhcode`, `rmccode` and `rmscode` are directly analogous except that a pcode value (≥ 101) is required, since Hopf bifurcation loci, period contours and stability boundaries are necessarily associated with parameter plane runs. Thus

```
rmhcode demo 107 102
```

deletes all files associated with the Hopf bifurcation locus with hcode 102 for pcode 107, while

```
rmscode 112 all
```

deletes all files associated with all stability boundaries, for pcode 112. The commands `rmbcode` and `rmecode` work in a similar way, but in this case a pcode value is never given since bifurcation diagram and eigenvalue convergence calculations are not associated with control parameter–wave speed planes. Thus

```
rmbcode demo 108
```

deletes all files associated with the bifurcation diagram with bcode 108, while

```
rmecode demo all
```

deletes all files associated with all eigenvalue convergence calculations.

To delete all files associated with a particular pcode, one can use the command `rmpcode`, for example

```
rmpcode demo 103
```

or

```
rmpcode demo 100
```

(the second of these will delete all files associated with any runs of `ptw`, `stability`, `bifurcation_diagram` and `eigenvalue_convergence`). The usage

```
rmpcode demo all
```

is also allowed; this will delete all output associated with the input subdirectory `demo`, and confirmation is requested to prevent unwanted deletion of a large amount of output.

3.1.7 Keeping Track of WAVETRAIN Runs

If one is doing a large number of different WAVETRAIN runs for the same problem, it can be a challenge to keep track of which run is which. A useful aid in this situation is the file `command.txt`, which is present in each output subdirectory corresponding directly to a WAVETRAIN command. For example, in §2.1.1, the command

```
hopf_locus demo 101 2.0 0.8 3.5 0.8
```

was used to calculate a Hopf bifurcation locus, and was allocated the hcode value 101. Then the file `command.txt` in the directory `output_files/demo/pcode101/hcode101/` contains a single line, in which the command is repeated. Further details of `command.txt`, and of other WAVETRAIN output files, are given in §4.4.1.

Runs of `ptw_loop` and `stability_loop` create a `command.txt` file in the pcode output directory, but not in the individual rcode subdirectories. To help keep track of the runs in this situation, WAVETRAIN has the command `list_rcodes`. This has one argument, a pcode value, and it lists the control parameter and wave speed associated with each rcode value for that pcode, plus the overall outcome of the calculation, and the period of the wave if one was found. If the argument is either omitted or is equal to 100, then the list corresponds to waves calculated individually, via either the `ptw` or `stability` commands.

3.1.8 The Parameter `iwave`

A major potential complication for calculations using WAVETRAIN is that there may be folds in the branch of periodic travelling wave solutions, implying that there is more than one wave solution for some pairs of control parameter and wave speed values. An example of this is provided by the files in the `demo1` input subdirectory. This problem has the same equations and the same values of the "other parameters" as for `demo`, but considers different ranges for the control parameter A and the wave speed c, and uses different settings in `constants.input`. Thus the input files in `demo` and `demo1` are identical except for `parameter_range.input` and `constants.input`. Looping through the control parameter–wave speed plane in the usual way using the `ptw_loop` command shows that periodic travelling wave solutions exist in a thin diagonal strip in this parameter plane. The results of the `ptw_loop` command for the `parameter_range.input` file provided at installation are illustrated in Figure 3.4a. Note that during this run and several of the subsequent runs for the problem `demo1`, a warning message about a small number of continuation steps will appear. This can be ignored: it is a consequence of the rather large step sizes that are set for the illustrative problems `demo` and `demo1`. Hopf bifurcation and homoclinic solution loci can be calculated in the usual way, via the commands

```
hopf_locus demo1 101 1.065 21.0 1.08 21.0
```

and

```
period_contour demo1 103 period=3000 1.085 20.0 1.08 20.0
```

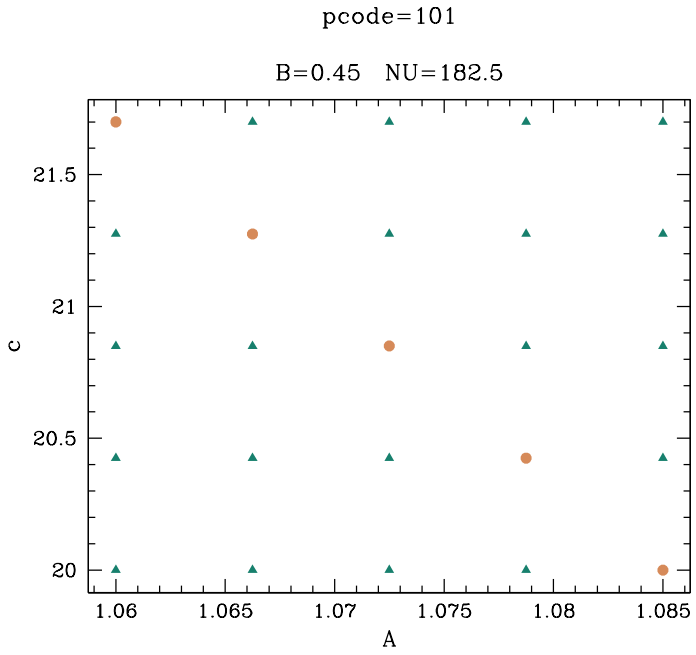
The results are illustrated in Figure 3.4b, showing that these loci intersect one another. This indicates a somewhat complicated solution structure, which is best investigated using the `bifurcation_diagram` command. Figure 3.5 illustrates a typical result from such a study, generated by the command

```
bifurcation_diagram demo1 c=20.2
```

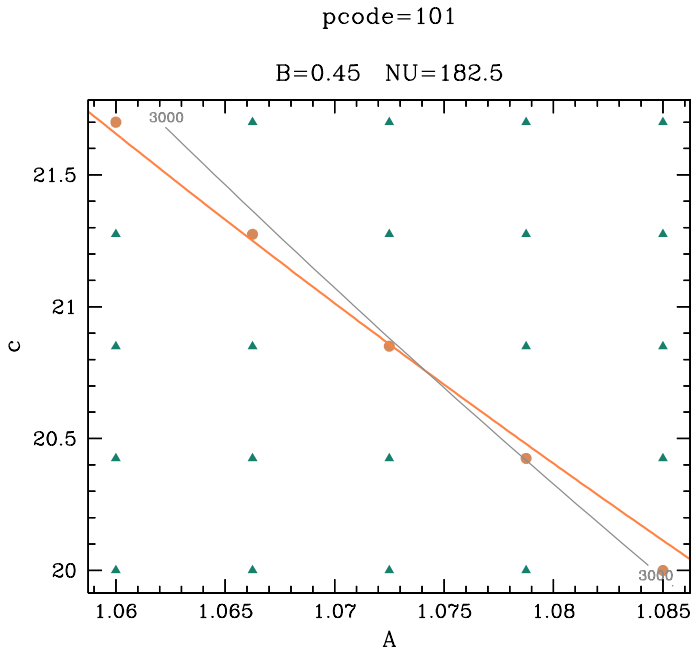
which shows that there is a fold in the periodic travelling wave solution branch, with two different periodic travelling wave solutions for some values of A.

When there are such multiple solutions, WAVETRAIN is able to study all of them via the parameter `iwave`. In all previous examples `iwave` has been set to 1, which causes WAVETRAIN to study the first wave solution along the solution branch for a given pair of A and c values. Here the counting of wave solutions is done as the control parameter varies, starting from the solution located by the wave search method specified in `equations.input`. Setting `iwave`=2 causes WAVETRAIN to study instead the second wave solution for the given parameters.

To illustrate this, Figure 3.6a shows the results of a run of `ptw_loop` for `demo1` for a finer grid of control parameter and wave speed values than used in Figure 3.4a, but again with `iwave`=1. To perform this run, `parameter_range.input` has been editted, with the grid reset to 50×15, but all other constants have been left as they were at installation. Note that these grid dimensions mean that `ptw_loop` attempts to calculated periodic travelling wave solutions for 750 pairs of control parameter and wave speed values, and consequently the run time for this command is relatively long (about an hour on a



(a)



(b)

Figure 3.4: (a) Results on the existence of periodic travelling wave solutions for the problem `demo1`. (b) The same plot as in (a) but with the addition of the Hopf bifurcation locus and the locus of (an approximation to) the locus of homoclinic solutions. A key illustrating the meaning of the various colours and symbols is shown in Figure 2.4 on page 19. The run and plot commands used to generate these figures are given in the main text, and are also listed in the Appendix.

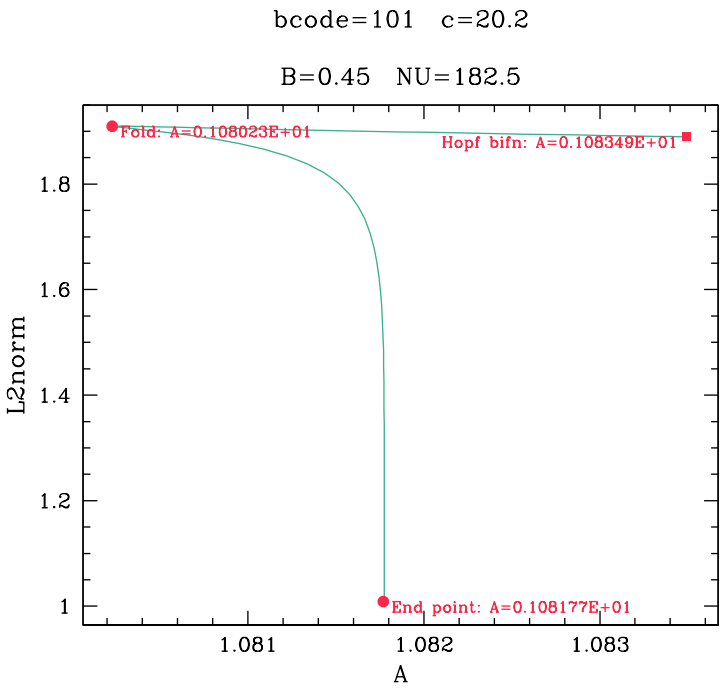
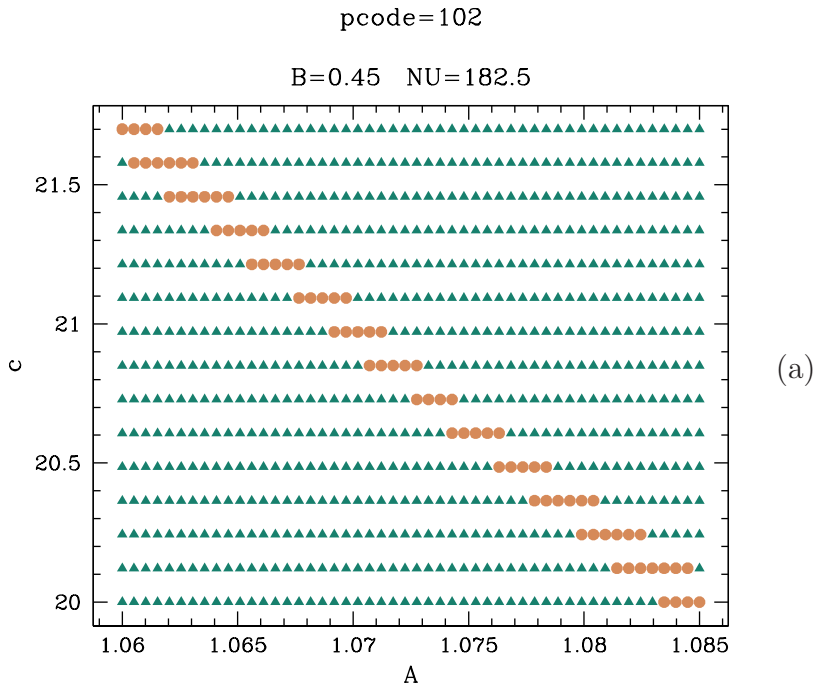


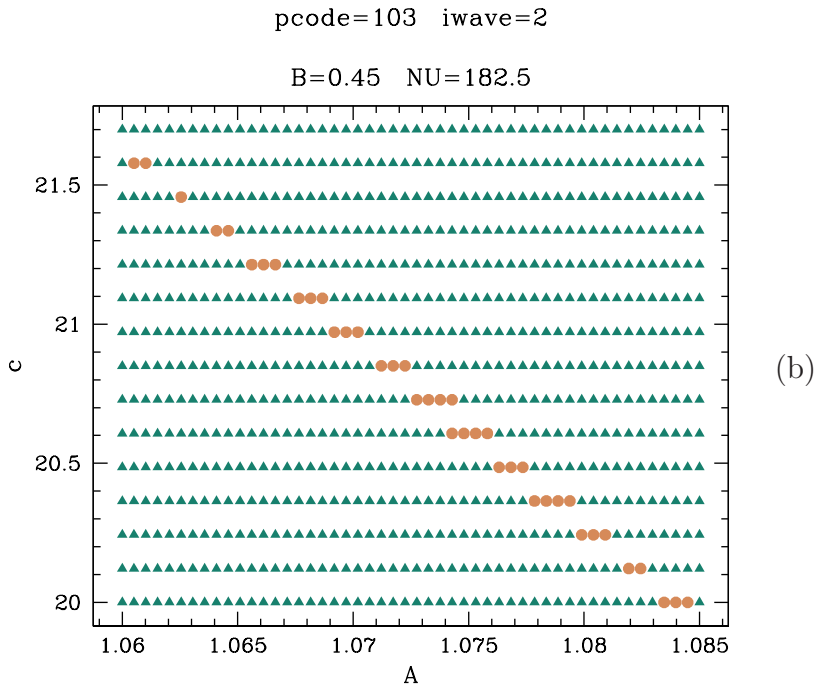
Figure 3.5: A typical bifurcation diagram for the problem `demo1`. The run and plot commands used to generate this figure are given in the main text, and are also listed in the Appendix.

typical desktop computer). In addition, the command `plot demo1 102` takes some time to perform its initial setups (about 5 minutes on a typical desktop computer) because of the large volume of data that is being processed. Figure 3.6a shows that there is a strip of the parameter plane in which there are periodic travelling wave solutions; the left hand boundary of this strip is composed partly of the Hopf bifurcation locus, partly of the homoclinic solution locus, and partly of the fold in the bifurcation diagram. (WAVETRAIN does not have the capacity to track the locus of such a fold).

If one edits the file `constants.input` and changes `iwave` to 2, and then reruns `ptw_loop`, one finds a thinner strip of the parameter plane in which there are periodic travelling waves (illustrated in Figure 3.6b). This strip is bounded by the locus of folds (on the left) and the homoclinic locus (on the right). This thin strip is the region of the parameter plane in which there are two different periodic travelling waves. If one were to proceed to calculate wave stability with `iwave` still set to 2, it is the stability of this second wave that would be calculated. Similarly, calculations done using the `period_contour` and `stability_boundary` commands would refer to the second wave along the solution branch. Setting `iwave` > 2 for `demo1` would simply show that there is no part of the parameter plane in which there are more than two periodic travelling waves.



(a)



(b)

Figure 3.6: Results on the existence of periodic travelling wave solutions for the problem `demo1`, using a fine grid of control parameter–wave speed values. (a) `iwave`=1; (b) `iwave`=2. A key illustrating the meaning of the various colours and symbols is shown in Figure 2.4 on page 19. The run and plot commands used to generate these figures are given in the main text, and are also listed in the Appendix.

The parameter `iwave` can also be set to zero. To illustrate the meaning of this special setting, consider the example problem `demo` discussed in §2.1. The selected region of the control parameter–wave speed plane has a significant region to the right of the Hopf bifurcation locus in which there are no periodic travelling wave solutions. If `iwave`=1, searching for a wave for control parameter and wave speed values in this region would proceed as follows. First, WAVETRAIN would vary the control parameter across the search region for Hopf bifurcations (specified in `equations.input`). If a Hopf bifurcation is detected, WAVETRAIN would then vary the control parameter along the periodic travelling wave solution branch, searching for the required value of the control parameter. However, since there is no periodic travelling wave solution, this search only ends when the numerical continuation ends because of a convergence failure close to the homoclinic solution locus. If one knew, or assumed, that the Hopf bifurcation was supercritical then one could eliminate this entire computation, since one would know *a priori* that there are no periodic travelling wave solutions to the right of the Hopf bifurcation locus. This assumption can be implemented by setting `iwave`=0. The file `equations.input` contains the start and end values of the range of control parameter values over which to search for a Hopf bifurcation in the travelling wave equations (see §2.2.2). The specific consequence of setting `iwave`=0 is that the end value is not used: it is replaced by the value of the control parameter at which a periodic travelling wave is sought. For the problem `demo`, if one edits `equations.input` changing `iwave` from 1 to 0 and then reruns the `ptw_loop` command (followed by calculation of Hopf bifurcation loci and period contours as in §2.1), the result is as shown in Figure 3.7; this should be compared with Figure 3.1 on page 76. The overall structure of the parameter plane is the same, but different outcome symbols are now used on the right and left hand sides of the region of periodic travelling waves. The blue-green triangles on the left hand side indicate that the search for a periodic travelling wave ended with a convergence failure in the numerical continuation. Typically this corresponds to the branch of periodic travelling wave solutions approaching a homoclinic solution, though of course it might indicate a real error. The new symbol (a purple square) indicates that the search for a periodic travelling wave ended without a convergence failure. This occurs most often when `iwave` has been set to 0 and no Hopf bifurcation is found, and this is the case for Figure 3.7. However, it could occur for other reasons, for example if the values of `ds`, `dsmin` and `dsmax` are too small, so that continuation ends prematurely (but without a convergence error). In all cases, more detailed information on the outcome of the run is available in the file `outcome.data` in the relevant output subdirectory (see §4.4); this indicates which of the different possibilities has occurred. Note that if the user wishes to include a key in material for presentation or publication, then they will probably prefer to use a single entry for cases where there is no periodic travelling wave, and correspondingly to have a single entry in the key. This can be achieved by changing the plotter setting `pplanekeytype` (see §3.3.1).

The key advantage of setting `iwave` to 0 is that the run time for the loop is lower. However, care must be exercised when using this setting, because it would give misleading results if the Hopf bifurcation was subcritical or had a fold.

Further details of the problem studied using `demo1` are given in Sherratt (2011b).

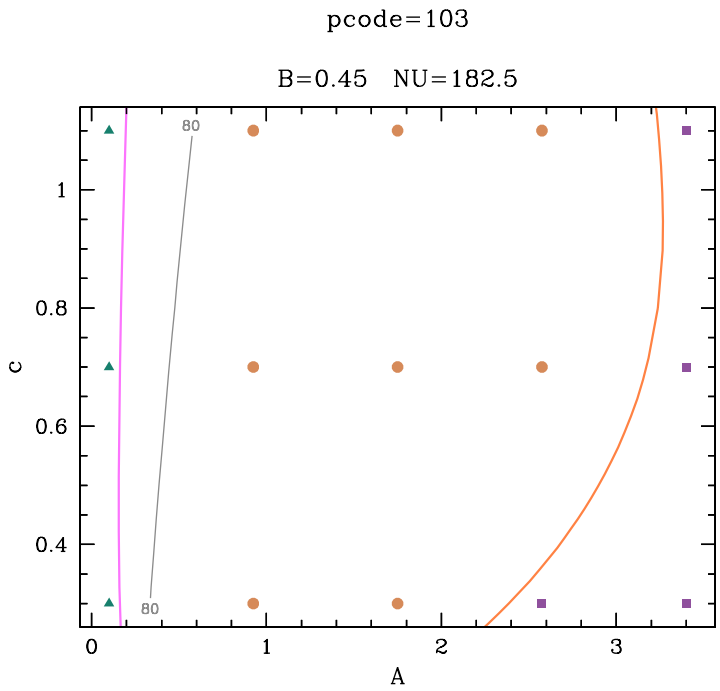


Figure 3.7: An illustration of the effect of setting the constant `iwave` to 0. This figure should be compared with Figure 3.1 on page 76, which shows the corresponding results for `iwave`=1. A key illustrating the meaning of the various colours and symbols is shown in Figure 2.4 on page 19. The run and plot commands used to generate this figure are given in the main text, and are also listed in the Appendix.

3.1.9 Setting the Wave Search Method and Hopf Bifurcation Search Range in Complicated Cases

As well as listing various equations, the file `equations.input` specifies the method used by WAVETRAIN to locate a periodic travelling wave for given control parameter and wave speed values. In many cases (such as for the problem `demo` discussed in §2.1) there is exactly one Hopf bifurcation in the travelling wave equations for any given value of the wave speed. Then a "direct" method can be used, meaning that WAVETRAIN searches for a Hopf bifurcation at the wave speed required for the periodic travelling wave, and then proceeds "directly", via a single numerical continuation, to the required wave solution. The control parameter range used in the Hopf bifurcation search is specified in the two lines following the word "direct" in `equations.input`. For `demo` a suitable search range has a starting value of $2.001B$, since the steady state undergoing the Hopf bifurcation only exists for $A \geq 2B$[†]. Here A is the name assigned to the control parameter in `variables.input`,

[†]The actual condition for steady state existence is $A \geq 2B$. However, there is a saddle-node bifurcation at $A = 2B$, with two steady states for $A > 2B$, only one of which is of interest in the problem `demo`.

and B is one of the parameters specified in `other_parameters.input`. The end value of the search range is 3.8, which is the upper limit on A in `parameter_range.input`; note however that the Hopf bifurcation search range is not restricted to the range specified in `parameter_range.input`.

The real importance of the Hopf bifurcation search range is for more complex situations in which there is more than one Hopf bifurcation as the control parameter is varied with a fixed wave speed. In the absence of an example problem that provides an adequate illustration of the various possibilities, this discussion is illustrated using a sketch (Figure 3.8). Suppose that for a particular problem, periodic travelling waves exist within the region of the control parameter–wave speed plane that is spotted in Figure 3.8a. For simplicity, assume that there is exactly one periodic travelling wave solution throughout this region, and that WAVETRAIN is being run with `iwave`=1 (see §3.1.8 for information on `iwave`). One might at first specify a direct wave search method with the Hopf bifurcation search range having a start value of 2.0 and an end value of 1.0. Running `ptw` or `spectrum` would then cause WAVETRAIN to stop at the first Hopf bifurcation it encountered as the control parameter decreased from 2.0 to 1.0, and to then continue travelling wave solutions from that point. This would lead to the detection of periodic travelling waves in the parameter region that is spotted in Figure 3.8b. Note that the order of the Hopf bifurcation search end points in `equations.input` is important. If instead one specified a search range with a start value of 1.0 and an end value of 2.0, the parameter region in which periodic travelling waves were detected would be the spotted region in Figure 3.8c.

Plotting the results from a study with either of these Hopf bifurcation search ranges would immediately suggest that an investigation using the `bifurcation_diagram` command would be helpful. Crucially, this command does not use the wave search method and Hopf bifurcation search range specified in `equations.input`. Rather, it scans the parameter range specified in `parameter_range.input` and continues the branch of periodic travelling wave solutions emanating from each Hopf bifurcation that is detected. Running `bifurcation_diagram` for a series of different values of the wave speed would reveal the true structure of the parameter plane, which could be clarified further by calculating the loci of Hopf bifurcation points and homoclinic solutions. This would show that there are regions of the control parameter–wave speed plane in which periodic travelling waves exist, but which are inaccessible to WAVETRAIN with a direct search method and a Hopf bifurcation search range with start and end values of 2.0 and 1.0. To calculate wave forms and stability in these regions, one would use a different Hopf bifurcation search range. For example, search range start and end values of 1.25 and 1.5 (in either order, and again with the direct wave search method) would enable WAVETRAIN to access periodic travelling wave solutions in the part of the control parameter–wave speed plane that is spotted in Figure 3.8d.

The term "direct" is used for the wave search methods discussed above because, once

To avoid WAVETRAIN following the wrong steady state branch when searching for a Hopf bifurcation, the problem `demo` has been formulated following the advice in the comments in `equations.input`, with the condition for steady state existence being set slightly away from the bifurcation point, specifically $A \geq 2.001B$. Correspondingly, the end point for the Hopf bifurcation search range is set to $A = 2.001B$ rather than $A = 2B$.

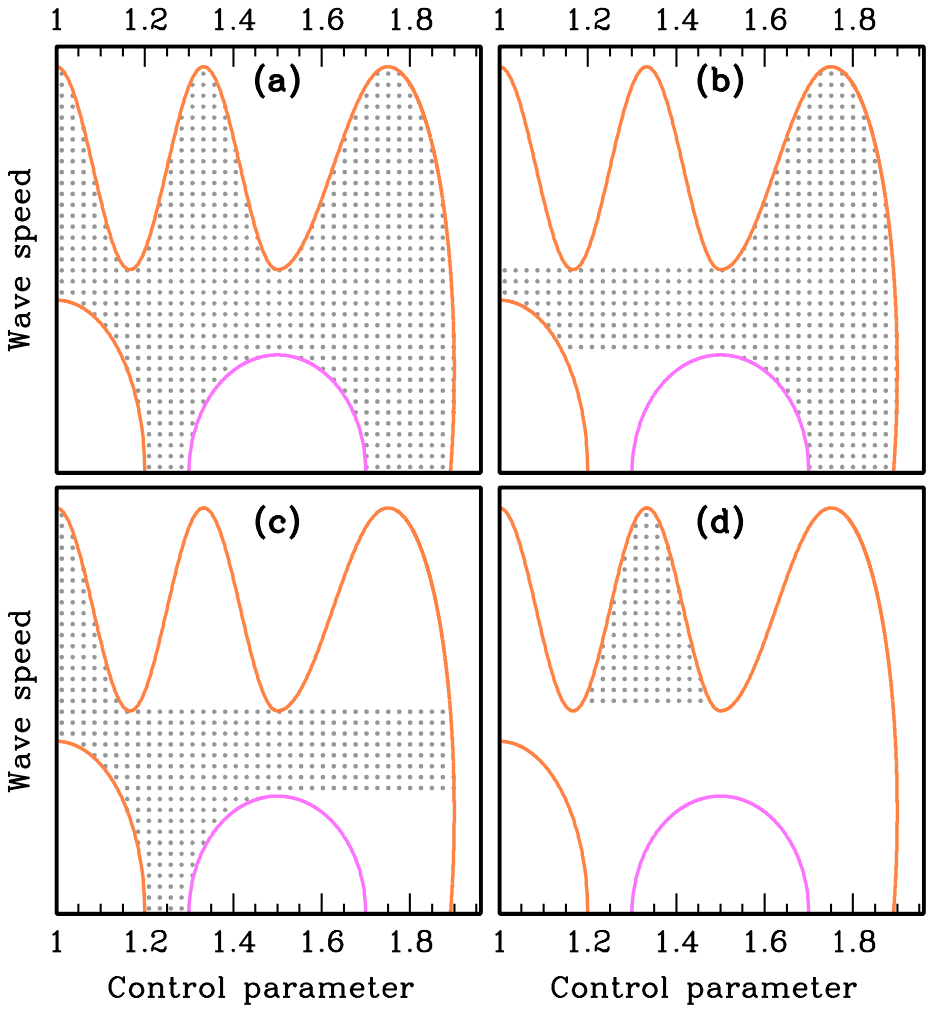


Figure 3.8: An illustration of the effects of changing the Hopf bifurcation search range, which is set in `equations.input`. This figure is a sketch. (a) The spotted region is the parameter region in which there are periodic travelling waves. For simplicity it is assumed that there is exactly one periodic travelling wave solution throughout this region, and that WAVETRAIN is being run with `iwave`=1 (see §3.1.8). (b–d) The spotted region is the parameter region in which periodic travelling waves are accessible to WAVETRAIN for three different Hopf bifurcation search ranges, using a "direct" wave search method in all three cases: (b) 1.95–1.0; (c) 1.0–1.95; (d) 1.25–1.5 or 1.5–1.25. The orange curves represent loci of Hopf bifurcations in the travelling wave equations, and the pink curves indicate loci of homoclinic solutions, as in the key in Figure 2.4.

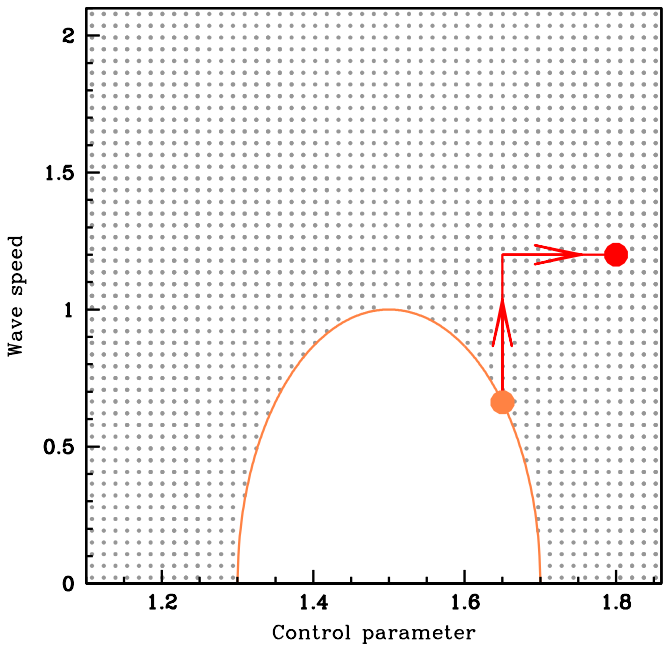


Figure 3.9: An illustration of an example requiring an "indirect" wave search method. This figure is a sketch. The spotted region is the parameter region in which there are periodic travelling waves. The orange curve represents a locus of Hopf bifurcations in the travelling wave equations, as in the key in Figure 2.4. The red lines indicate the wave search method, which starts from a Hopf bifurcation at the point indicated by the large orange dot, and proceeds first with a constant control parameter value and then with a constant wave speed, reaching the required values (indicated by the large red dot) "indirectly".

the Hopf bifurcation point has been found, WAVETRAIN locates the periodic travelling wave in a single numerical continuation, simply varying the control parameter along the periodic travelling wave solution branch until the required value is reached. However, there are some situations in which this simple approach cannot be used, and an example is illustrated in the sketch in Figure 3.9. Again periodic travelling waves exist within the region of the control parameter–wave speed plane that is spotted. For values of the wave speed less than 1, the periodic travelling waves can easily be located using a "direct" search method, as discussed above. However for wave speeds greater than 1, there is no Hopf bifurcation for any value of the control parameter, and thus this method cannot be used. WAVETRAIN offers the "indirect" search method for this situation. Here the Hopf bifurcation search occurs by varying the wave speed within a specified range, at a specified value of the control parameter. For instance, suppose that one wished to study

a periodic travelling wave for control parameter 1.8 and wave speed 1.2, illustrated by the large red dot in Figure 3.9. The user might specify a Hopf bifurcation search between wave speeds 0.5 and 0.8, at control parameter value 1.65. WAVETRAIN would then find the Hopf bifurcation point indicated by the large orange dot in Figure 3.9. It would then perform two separate numerical continuations to locate the required wave. Firstly the periodic travelling wave solution branch would be followed, varying the wave speed with the control parameter fixed, until the required value is reached. Then the control parameter would be varied, with fixed wave speed, until the required pair of values is reached.

One or other of the direct and indirect wave search methods is will work provided that there are Hopf bifurcations of the travelling wave equations somewhere in the control parameter – wave speed plane. However, it is possible that there is not a Hopf bifurcation for any pair of control parameter and wave speed values. To accommodate this situation, WAVETRAIN provides a third wave search method, termed the "file" method. In this case, the user must supply a periodic travelling wave solution for one pair of control parameter and wave speed values; typically this would come from numerical simulations of the partial differential equations. The control parameter and wave speed values for this solution are given in `equations.input`, and the solution itself is specified in the additional input file `ptwsoln.input`, which must be placed in the relevant input subdirectory. The required format for `ptwsoln.input` is described in §2.2.2. Using this solution as a starting point, WAVETRAIN first follows the periodic travelling wave solution branch with the control parameter fixed, varying the wave speed until the required value is reached. Then the control parameter is varied, with fixed wave speed, until the required pair of values is reached.

An important warning must be given concerning the value of the initial step size `ds` (specified in `constants.input`) when using the indirect or file methods. In these cases, calculation of the required periodic travelling wave usually involves two separate continuation stages, the first varying the wave speed with a constant control parameter value, and the second varying the control parameter with a constant wave speed value. However, if the control parameter value for the required wave is the same as that specified in `equations.input` for the Hopf bifurcation search (indirect method) or for the solution in `ptwsoln.input` (file method), then the second continuation stage is omitted. In fact, it is omitted even if the two control parameter values differ, but only slightly; the threshold difference for doing the second stage is determined by the constants `controlatol` and `controlrtol`, which are set in `defaults.input`. If the difference between the two control parameter values is small but exceeds the threshold, then WAVETRAIN may fail to find the required periodic travelling wave because the first continuation step is too large, causing the numerical continuation to "jump over" the required point. The remedy for this is to reduce the initial continuation step size, `ds`, and also the minimum step size `dsmin` if this is necessary in order that `ds`$\geq$`dsmin`. The constants `ds` and `dsmin` are set in `constants.input`, and the relevant values are those in the second line of step size settings. It is recommended that relatively small values of these two constants are used in conjunction with the indirect or file wave search methods.

A single wave search method can be used for all control parameter and wave speed values, but the method and/or the Hopf bifurcation search range can be parameter-

dependent. Thus in order to cover the whole of the part of the control parameter – wave speed plane illustrated in Figure 3.9, the relevant part of `equations.input` could read as:

```
# Wave search method and Hopf bifurcation search range
c<1 & P>1.5
  direct
  1.5
  1.8
c<1 & P<1.5
  direct
  1.5
  1.2
c>=1
  indirect :  P=1.65
  0.5
  0.8
```

where `P` and `c` are the names for the control parameter and wave speed respectively, set in `variables.input`. In this example all of the start and end values, and all of the inequality limits, are constant. However they can depend on the control parameter and wave speed, and also on the parameters defined in `other_parameters.input`. Note that although a mixed search method such as this can involve the "file" method, only one reference pair of control parameter and wave speed values can be used, since only one `ptwsoln.input` file is permitted.

An example illustrating the different search methods is provided in the problem `demo2`. This is identical to `demo` except for two changes. Firstly, the single wave search method specified in `equations.input` for `demo` has been replaced by a more complicated mixed method, in which direct, indirect and file methods are used in different parts of the control parameter–wave speed plane. Secondly, the values of `ds` and `dsmin` for the continuation of periodic travelling waves have been reduced, as recommended on page 91 for the indirect and file methods. For the "file" case, a suitable wave solution has been provided in the `demo2` subdirectory of `input_files`. This solution was actually constructed from a WAVETRAIN output file, although in a real problem, output from a numerical simulation of the partial differential equations would normally be used. Entering the command

```
ptw_loop demo2
```

performs a loop across the parameter plane for this problem. One can plot the results in the usual way, by typing

```
plot demo2 101
```

(the number 101 is the pcode value) and then

```
@pplane
```

at the plotter prompt. If the default plot type is selected by entering RETURN (ENTER) when prompted, Figure 2.3 is reproduced. The plotter can then be exitted in the usual way (`@exit` or `@quit`).

Finally, it is important to comment on the use of the parameter `iwave` with the different search methods. The setting `iwave`=0 can only be used in the direct case. Settings of `iwave`> 1 are unaffected by the choice of direct, indirect or file search method, with one exception. If a periodic travelling wave is required at a value of the control parameter that is the same as that specified for the Hopf bifurcation search in the indirect case, or for the control parameter value corresponding to the solution in `ptwsoln.input` in the file case, then the wave is calculated in a single continuation step, varying the wave speed: the continuation that would usually be done in the control parameter is not required. Therefore the calculation does not provide WAVETRAIN with a direction of travel along the periodic travelling wave solution branch for fixed wave speed. Hence settings of `iwave`> 1 are not possible, and will cause WAVETRAIN to terminate the run with an error message.

3.1.10 Details of the Matrix Eigenvalue Calculation

The first step in determining periodic travelling wave stability is to calculate the eigenvalues corresponding to periodic eigenfunctions, which form starting points for numerical continuation of the eigenvalue spectrum. WAVETRAIN does this by replacing the derivatives (with respect to the travelling wave variable) in the eigenvalue equation by finite difference approximations, with periodic boundary conditions on a domain of length equal to one period of the wave. The order of these approximations is determined by the constant `order`, set in `constants.input` (see §2.2.1). The resulting matrix eigenvalue problem is solved using routines from version 3.1.1 of LAPACK (Anderson *et al.*, 1999), and the associated routines from BLAS (Lawson *et al.*, 1979; Dongarra *et al.*, 1988a,b; Dongarra *et al.*, 1990a,b). Further details of these packages are available from `www.netlib.org/lapack` and `www.netlib.org/blas` respectively. If the equations being studied are of the form (1.1a), meaning that each of equation contains a time derivative, then the eigenvalue problem if of standard type, and is solved using the LAPACK routine `dgeevx`. However if the equations are of the form (1.1b,c), meaning that there is no time derivative in one or more of the equations, then the eigenvalue problem is of generalised type, and is solved using the LAPACK routine `dggevx`. In fact, in this latter case it is possible to convert the eigenvalue problem into one of standard type (Sherratt, 2011a), and future versions of WAVETRAIN may adopt this approach. However the coding changes required to use `dggevx` rather than `dgeevx` are very slight, and on these grounds WAVETRAIN currently adopts this less efficient approach.

LAPACK makes extensive use of the Basic Linear Algebra Subprograms (BLAS). To maximise computational speed when using LAPACK, one should use a BLAS library that is optimised for the particular computer being used. However, in the absence of such a library, there is a Fortran77 reference implementation of the BLAS, and this is supplied with WAVETRAIN. Users of WAVETRAIN are recommended to use this reference implementation unless they already have an optimised BLAS library, since LAPACK computations usually constitute only a small part of the run times for WAVETRAIN. However if users are interested in installing an optimised BLAS library, they should consult `www.netlib.org/blas` or the Wikipedia entry on BLAS. Once a user has their own BLAS library, it is incorporated

into WAVETRAIN via the `blas` entry in `defaults.input` (see §3.2 for details).

Provision of a specific BLAS library by the user raises one small technical difficulty. There is a Fortran77 function `LSAME` that is used by both LAPACK and BLAS. The user's BLAS library may or may not include this function. If it does, then WAVETRAIN's version of `LSAME` must be excluded from the relevant Fortran77 compilations, and this is does via the `lsame` entry in `defaults.input` (see §3.2 for details).

Another issue of a similar type concerns the LAPACK function `DLAMCH`. This returns the value of "machine epsilon", which gives a bound on the roundoff in individual floating-point operations. A version of this function is distributed with LAPACK (version 3.1.1), and this is supplied with WAVETRAIN. This function will work on the vast majority of computers, but not all. In the latter case, the user will have to provide their own version of `DLAMCH`; see the LAPACK documentation for information about this. A user-supplied version of `DLAMCH` can be incorporated into WAVETRAIN via provision of the file name (including full path) in the `dlamch` entry in `defaults.input` (see §3.2 for details).

The computed eigenvalues will differ from the true eigenvalues corresponding to periodic eigenfunctions for two separate reasons: error in the calculation of the matrix eigenvalues, and differences between the discretised and actual eigenfunction equations. The first of these is monitored by WAVETRAIN, which determines estimated error bounds for each of the calculated eigenvalues. It is important to clarify that these bounds refer to errors in the calculation of the matrix eigenvalues, rather than the errors of the calculated values as solutions of the actual eigenfunction equation. The estimated error bounds depend on whether the equations being studied are of the form (1.1a) or (1.1b,c). In the former case, the bound is simply the quantity `EERRBD` that is calculated by the relevant code fragment in the LAPACK user's guide (Anderson *et al.*, 1999), and is an approximate bound on the absolute value of the difference between the actual and computed matrix eigenvalues. However the latter case, in which a generalised eigenvalue problem is solved, is somewhat more complicated. The corresponding code fragment in the LAPACK user guide provides a bound on the "chordal distance" between the actual eigenvalue (λ, say) and the computed eigenvalue ($\hat{\lambda}$, say),

$$\chi\left(\lambda,\hat{\lambda}\right)=\frac{\left|\lambda-\hat{\lambda}\right|}{\left(1+|\lambda|^2\right)^{1/2}\left(1+\left|\hat{\lambda}\right|^2\right)^{1/2}}\,.$$

For the purposes of WAVETRAIN, it is most useful to calculate instead a quantity that is an approximate bound on the error in the eigenvalue itself, and thus WAVETRAIN calculates

$$\left(1+\left|\hat{\lambda}\right|^2\right)\chi\left(\lambda,\hat{\lambda}\right).$$

This will be a crude approximation to an error bound on the eigenvalue provided that the relative error is not too large, but users should be aware of its limitations. Of course, the user can back-calculate the chordal distance bound if desired, using WAVETRAIN's crude estimate and the real and imaginary parts of the eigenvalue.

The error bounds for the matrix eigenvalues are written to the screen as part of the output from the `convergence_table` command, which is a vehicle for displaying the

results of calculations done by the `eigenvalue_convergence` command (see §2.1.2). They are also written to the `info.txt` file for calculations of wave stability (see §2.5 and §4.4.2), and are listed in the file `evalues.data` in corresponding rcode output subdirectory (see §4.4.7).

One further important point concerning errors in the matrix eigenvalues is that the estimated error bounds are provided simply for information. Future versions of WAVETRAIN may provide alternative methods for calculating the matrix eigenvalues that could be used if the errors are too large, but this facility is not currently available.

The differences between the discretised and actual eigenfunction equations can usually be reduced simply by increasing the number of points in the discretisation, which is achieved by increasing `nmesh2`, which is set in the file `constants.input`. The command `eigenvalue_convergence` (see §2.1.2) facilitates the selection of a suitable value of `nmesh2`. Typically, as `nmesh2` increases the matrix eigenvalues converge to the functional eigenvalues. This is guaranteed by analytical convergence results in many cases (Atkinson, 1964; Kreiss, 1972; de Boor & Swartz, 1980; Chatelin, 1981), but for some equations more complicated behaviour can occur. An example of this can be obtained by editting the file `constants.input` for the problem `demo` as follows:

- change `nmesh1` to 160
- change `nevalues` to 20 (leaving `iposre`=1).

Having made these changes, one can enter the command

```
eigenvalue_convergence demo 2.2 0.7 50 100 150 200 250 300 350 400 450 500
```

(run time: about 2 hours on a typical desktop computer). Investigation of the results using the `convergence_table` command shows that the first four matrix eigenvalues converge in a straightforward manner to the corresponding functional eigenvalues. However for the fifth functional eigenvalue the situation is more complicated. There is a sequence of matrix eigenvalues that converges to this functional eigenvalue, as illustrated in Figure 3.10. However the appropriate matrix eigenvalue is only number 5 for relatively small `nmesh2` values. As `nmesh2` is increased above 100, additional matrix eigenvalues appear with real parts in between those of the fourth and fifth functional eigenvalues, and with very large imaginary parts ($\sim 10^4$). These eigenvalues appear to be an artifact of the discretisation. In a case such as this it is convenient to exclude matrix eigenvalues with very large imaginary parts from those used as starting points for numerical continuation of the spectrum. This can be achieved using the constant `evibound`, set in `defaults.input` (see §3.2).

Even when the matrix eigenvalues converge in a simple manner to the functional eigenvalues, it is typical that the numerical error bounds on their calculated values increases. This is because the condition number of the matrix increases as one of its eigenvalues approaches zero, which is always a functional eigenvalue.

An appropriate choice of `nmesh2` will be a compromise between these various trends, with the smallest viable choice being optimal to reduce run times. Moreover in difficult cases, setting the constant `order` to a value greater than one may enable a smaller value of `nmesh2` to be used; examples of this are given in §2.3 and at the end of §3.1.11.

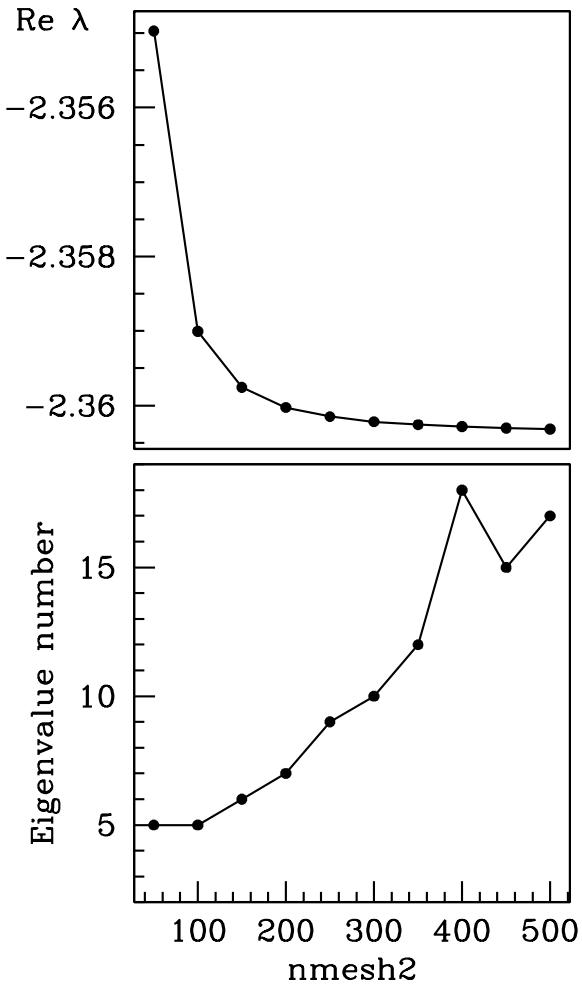


Figure 3.10: An example of a complicated pattern of convergence to a functional eigenvalue of the eigenvalues of the matrix given by discretising the eigenfunction equation in the travelling wave coordinate. This figure was not itself generated by WAVETRAIN, but the data that is plotted was generated by the `eigenvalue_convergence` command for an amended version of the problem `demo`, as described in the main text. After the run of this command, the command `convergence_table` was run for each of the eigenvalues numbered 5-18 (individually). In each case the table was examined for eigenvalues close to $-2.3603 + i * 0.9935$ (real and imaginary parts both within 0.1 would be a suitable criterion). Any such eigenvalues are plotted against the corresponding `nmesh2` value in the upper panel, and the corresponding eigenvalue number(s) are plotted against `nmesh2` in the lower panel. The results show that as the discretisation becomes finer, new matrix eigenvalues with real parts between those of the fourth and fifth functional eigenvalues appear; these eigenvalues all have very large imaginary parts ($\sim 10^4$) and appear to be an artifact of the discretisation.

Finally it is important to note that differences between the matrix and functional eigenvalues, whatever their cause, do not translate at all into errors in the calculated eigenvalue spectrum. All that is required is that the calculated matrix eigenvalues are sufficiently close to the functional eigenvalues that they provide a starting point from which numerical continuation can proceed. In reality the numerical continuation is typically very tolerant of poor starting approximations.

3.1.11 An Outline of How the `stability_boundary` Command Works

Although its syntax is not particularly complicated, the internal workings of the command `stability_boundary` are much more complex than those of the other WAVETRAIN commands. Of course the user does not need to be concerned with this, but it is helpful to understand the basic way in which the command operates, in order to make sense of the messages that are written to the screen and/or the `info.txt` file during a run. The description in this section will be deliberately brief: full details of the computational algorithms are given in Rademacher *et al* (2007) and Sherratt (2011c).

A brief summary of the mathematical background will be helpful to many users. Stability changes of periodic travelling waves can be of either Eckhaus or Hopf type (Rademacher & Scheel, 2007). Recall that the eigenvalue spectrum of a periodic travelling wave always passes through the origin, corresponding to neutral stability to translations. Also, the spectrum will always be symmetric about the real axis. A change of stability of Eckhaus type occurs when the curvature of the spectrum at the origin changes sign (illustrated schematically in Figure 3.11a). This was the type of stability change that occurred in the problem `demo`, discussed in §2.1. The alternative possibility is that the spectrum passes through the imaginary axis away from the origin (illustrated schematically in Figure 3.11b). This type of stability change is referred to as being of Hopf type.

Recall that the `stability_boundary` command has six compulsory arguments, which are the input subdirectory name and the pcode value, followed by two pairs of control parameter and wave speed values; these may be followed by optional arguments (see §3.1.2). The command operates via the following stages.

Stage 1: Calculation of the periodic travelling wave for the control parameter and wave speed given in arguments 3 and 4. The value of `iwave` is used to determine which wave solution is being considered, in the case of multiple solutions (see §3.1.8).

Stage 2: Calculation of the eigenfunction corresponding to the zero eigenvalue, again for control parameter and wave speed given in arguments 3 and 4. WAVETRAIN does this by calculating the eigenvalues corresponding to periodic eigenfunctions via discretisation (see §3.1.10). The matrix eigenvalue with smallest modulus is interpreted as an approximation to the zero functional eigenvalue. Using this approximation as a starting point, WAVETRAIN performs a numerical continuation in a dummy parameter, which generates a numerical solution of the eigenfunction equation.

Stage 3: Calculation of the first and second derivatives of the eigenvalue and eigenfunction with respect to γ for the zero eigenvalue, again for control parameter and wave speed

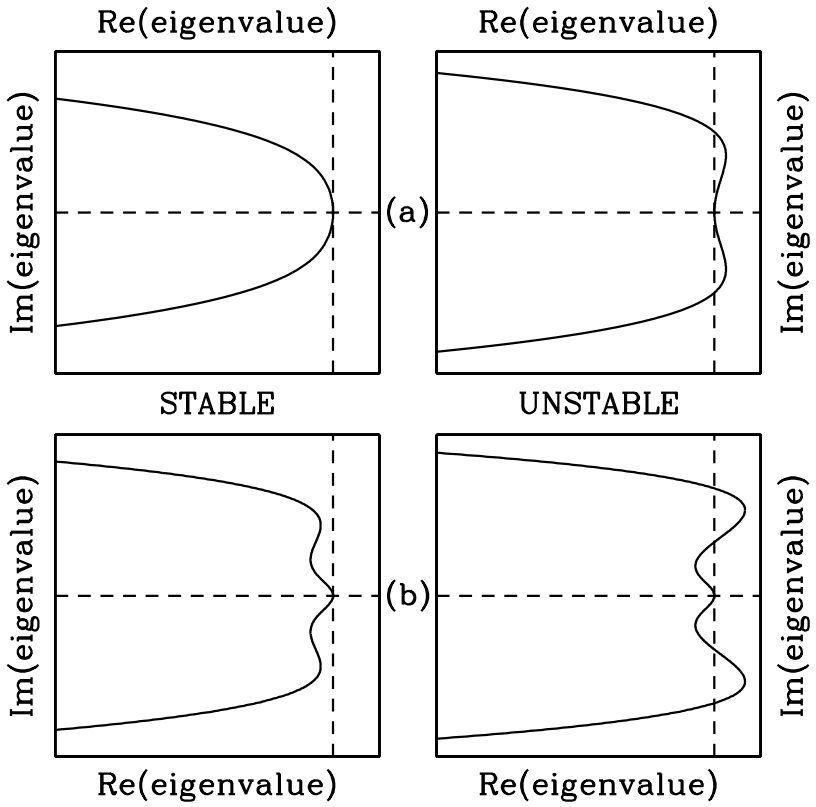


Figure 3.11: An illustration of the two different ways in which the stability of a periodic travelling wave can change. (a) and (b) show typical forms of the eigenvalue spectra on the stable (left) and unstable (right) side of a change in stability of (a) Eckhaus type and (b) Hopf type. The dashed lines denote the zero axes of the real and imaginary parts of the eigenvalue.

given in arguments 3 and 4. Here, as previously, γ is the phase difference in the eigenfunction across one period of the periodic travelling wave.

Stage 4: Numerical continuation of the periodic travelling wave, the eigenfunction for the zero eigenvalue, and the first and second derivatives of this eigenvalue and eigenfunction with respect to γ, as the control parameter/wave speed is varied between the value in arguments 3/4 and the value in arguments 5/6, with the wave speed/control parameter fixed at the common value of arguments 4 and 6 / 3 and 5. (Recall that either arguments 3 and 5 or arguments 4 and 6 must be the same.) During this continuation, WAVETRAIN monitors the value of the real part of the second derivative of the eigenvalue with respect to γ, looking for a zero, which would correspond to a change of stability of Eckhaus type. If such a stability change is detected, the command progresses to Stage 5A; if not, the next step is Stage 5B.

Stage 5A: If a zero of the real part of the second derivative of the zero eigenvalue with

respect to γ is detected during Stage 4, then this zero point is continued numerically in the control parameter – wave speed plane, thereby tracing out the stability boundary. Since the initial zero point is in the interior of the region of the control parameter – wave speed plane under consideration, this continuation must be performed twice, with opposite initial directions. The command then ends.

Stage 5B: If a zero of the second derivative of the zero eigenvalue with respect to γ is not detected during Stage 4, WAVETRAIN concludes that the change of stability is of Hopf rather than Eckhaus type. WAVETRAIN then calculates the eigenvalue spectrum of the periodic travelling wave with control parameter and wave speed values given in arguments 3 and 4. Note that the eigenvalues with $\gamma = 0$, which form the starting point of this calculation, have been calculated previously in Stage 2.

Stage 6: Provided that the control parameter and wave speed values are sufficiently close to a stability change of Hopf type, the eigenvalue spectrum will contain at least one point with strictly positive imaginary part at which there is a fold, meaning that the slope of the spectrum is infinite (see Figure 3.11b). WAVETRAIN estimates the approximate location of the fold with positive imaginary part and largest real part via interpolation along the calculated spectrum. It then refines this estimate via numerical continuation of the equations for the periodic travelling wave, the eigenfunction, and the first derivative of the eigenvalue and eigenfunction with respect to γ. This relatively time-consuming continuation is performed over a small region of the spectrum containing the estimated fold location, and the size of this small region is determined by the constant `gatol`, set in `defaults.input`.

Stage 7: The fold located in Stage 6 is tracked numerically as the control parameter/wave speed is varied between the values in arguments 3/4 and 5/6, with the wave speed/control parameter fixed at the common value of arguments 4 and 6 / 3 and 5. (Recall that either arguments 3 and 5 or arguments 4 and 6 must be the same.) During this continuation, WAVETRAIN monitors the real part of the eigenvalue, looking for a point at which it is zero; this corresponds to a stability change of Hopf type, and will occur provided the initial control parameter and wave speed values are sufficiently close to the stability change.

Stage 8: The zero of the real part of the eigenvalue is continued numerically in the control parameter – wave speed plane, with its derivative with respect to γ also fixed at zero. This traces out the stability boundary. Since the initial zero point is in the interior of the region of the control parameter – wave speed plane under consideration, this continuation must be performed twice, with opposite initial directions.

At the end of Stage 8 the command ends. However, if a problem occurs during any of Stages 5B–8, WAVETRAIN calculates the periodic travelling wave and eigenvalue spectrum for the control parameter and wave speed values given in arguments 5 and 6, and then repeats Stages 6–8. This repetition is useful in case the algorithm works for the point given by arguments 5 and 6, but fails for the point given by arguments 3 and 4 because it is too far from the stability boundary. For example, there may not be a fold in the

spectrum, other than zero, if one is sufficiently far from the stability boundary on the stable side.

A simple example of a change in stability of Hopf type is discussed by Bordiougov & Engel (2006), and the `demo3` input subdirectory contains files that enable their equations to be studied using WAVETRAIN. One important difference between this problem and `demo` and `demo1` is that there is no algebraic formula for the homogeneous steady state from which periodic travelling waves arise. Therefore the input files must be augmented by a file `steadystate.input`, which lists the steady state values of the travelling wave variables at a series of values of the control parameter. This file must be generated by some external software, and for `demo3` this was done by the Fortran77 program `create_stst_file.f`; for the user's information, this program is provided in the `input_files/demo3` directory, but there is no need to run it since the `steadystate.input` file is also provided. In the part of the `equations.input` file corresponding to the steady states, one simply puts the word `file` (or `File` or `FILE`), and WAVETRAIN will then use `steadystate.input`. The command

```
stability_loop demo3
```

(run time: about six hours on a typical desktop computer) scans a region of the control parameter – wave speed plane. During the run, a warning about the value of `controlatol` appears for each pair of control parameter and wave speed values considered. This is because of the small numerical values of the control parameter in `demo3`. In view of this, it would be sensible to either reformulate the equations using the parameter $\widehat{\phi} = 10^4\phi$, or decrease `controlatol` (set in `defaults.input`). However the current settings do not cause any problems in practice and for demonstration purposes it is more convenient to retain them. Since this is the first run for `demo3`, it will be allocated the pcode value 101, and one can plot the results by typing

```
plot demo3 101
```

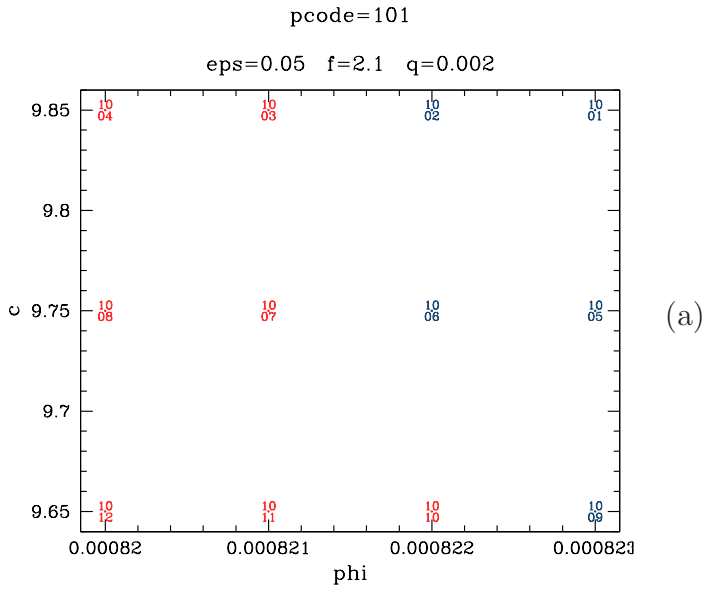
followed by the plotter command `@pplane`, selecting the default (`rcode`) option for the plot style. The result is illustrated in Figure 3.12a and reveals both stable and unstable periodic travelling waves. For example, the periodic travelling wave for $\phi = 8.21 \times 10^{-4}$, $c = 9.75$ is stable, while that for $\phi = 8.22 \times 10^{-4}$, $c = 9.75$ is unstable, and these points provide good starting points for tracing the stability boundary. To do this, one exits the plotter by typing `@exit` or `@quit`. One then runs the command

```
stability_boundary demo3 101 8.21E-4 9.75 8.22E-4 9.75
```

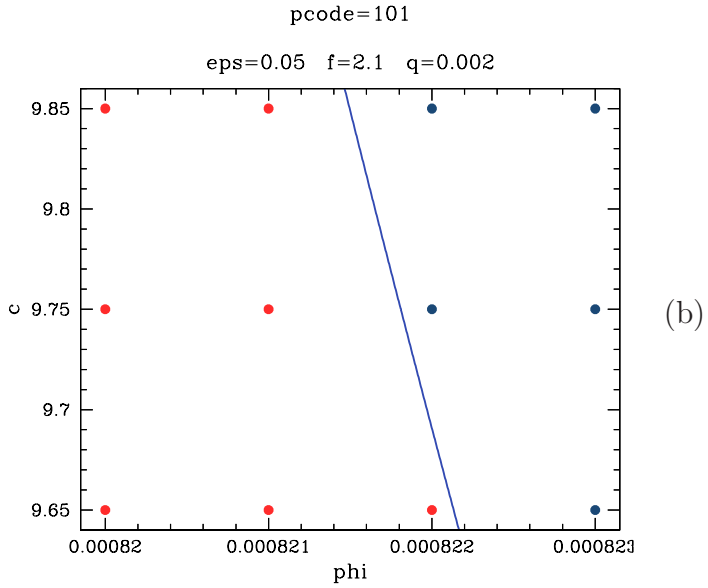
which moves progressively through each of the 8 stages described above (run time: about 90 minutes on a typical desktop computer). Various messages appear on the screen during the run to update the user on the progress of the calculation. Included amongst these is a warning about a small number of continuation steps, which results from the point $\phi = 8.21 \times 10^{-4}$, $c = 9.75$ being very close to the stability boundary. The warning about the value of `controlatol` also appears. Both of these warnings can be ignored.

To plot the result of this calculation, one re-enters the plotter by typing

```
plot demo3 101
```



(a)



(b)

Figure 3.12: Results on the stability of periodic travelling wave solutions for the problem `demo3`. (a) The results of a loop over a grid of points in the control parameter – wave speed plane. (b) The same results with the boundary between stable and unstable waves superimposed. The colour of this boundary shows that the stability change is of Hopf type (see Figure 2.4). The run and plot commands used to generate these figures are given in the main text, and are also listed in the Appendix. The quantities eps, f and q referred to in the second line of the title are parameters which appear in the equations but which are not being used as the control parameter; their values are specified in the file `other_parameters.input` (see §2.2.3).

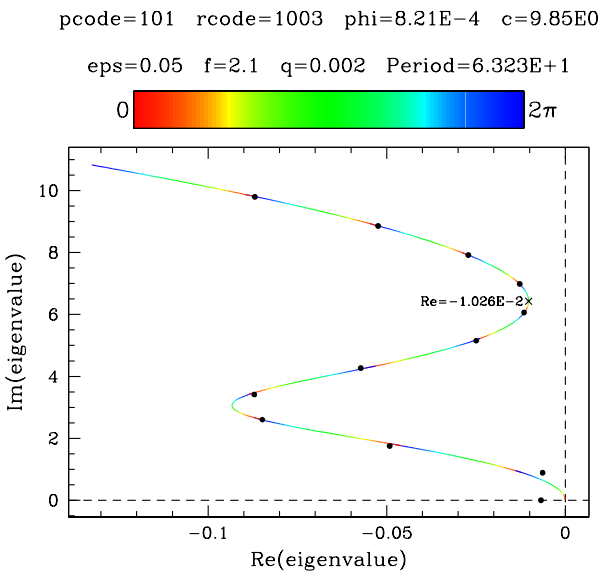
and then regenerates the results of the `stability_loop` run via the plotter command `@pplane`, in this case selecting the "symbol" plot style for variety. The stability boundary can then be superimposed on this plot by typing

```
@stability_boundary 101
```

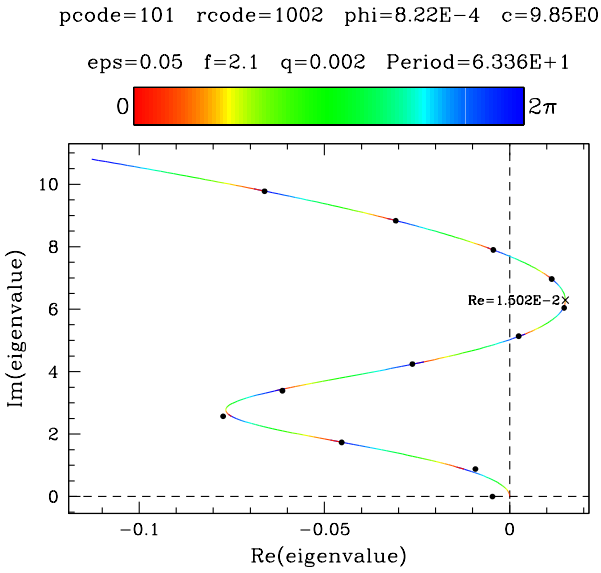
giving the result illustrated in Figure 3.12b. The colour of the stability boundary shows that it is of Hopf rather than Eckhaus type (see Figure 2.4). To see the change in the eigenvalue spectrum as the boundary is crossed, one can type `@spectrum 1003` and then `@spectrum 1002`, giving the eigenvalue spectra illustrated in Figures 3.13a,b. This demonstrates clearly that the change in stability arises from the spectrum crossing the imaginary axis away from the origin. The plotter can be exitted by typing `@exit` or `@quit`.

One important warning about the `stability_boundary` must be given, concerning step size in the case of a change in stability of Hopf type. Any numerical continuation calculation requires that the step size be sufficiently small in order for the calculation to be successful. There is no *a priori* means of knowing how small will be "sufficiently small" in a particular case. Numerical continuation of a stability boundary of Hopf type is defined by the conditions that the real part of the eigenvalue, and the real part of its derivative with respect to γ, are both zero. As well as holding (away from the origin) at a change in stability of Hopf type, these conditions both hold at the origin for the spectrum of any periodic travelling wave. Therefore if too large a step size is used, the continuation step can erroneously locate the origin, or a point close to it. Once the continuation has veered of in this way, the boundary-tracking algorithm will trace out a more or less random path in the parameter plane. In view of this it is important to check that the stability boundary remains on track throughout the calculation. This can be done either via a run of `stability_loop`, or by using `stability` to calculate the spectrum at a series of points along the stability boundary. In the latter case, appropriate pairs of control parameter and wave speed values can be obtained either via the optional arguments to the `stability_boundary` command (see §3.1.2) or by inspection of the output file `stabilityboundary.boundarydata` in the relevant scode output directory (see §4.4.8). If the calculation has veered off, the remedy is to reduce the step sizes `ds`, `dsmin` and `dsmax` (set on line 9 of `constants.input`) and rerun the `stability_boundary` command.

To conclude this section, I comment on a difference between `demo3` and `demo`, `demo1` and the previous problems `demo2`, namely that the constant `order` (set in `constants.input`) is set to 2 rather than 1. This constant specifies the order of the finite difference approximation used for the highest derivative when discretising the eigenfunction equation. Thus setting `order` = 1 causes WAVETRAIN to use a three-point approximation for the second derivative, while `order` = 2 gives a five-point approximation. In simple cases one would certainly use `order` = 1, but the higher level of accuracy resulting from `order` > 1 can be useful when convergence of the eigenvalues is slow as the number of mesh points (determined by `nmesh2`) is increased. The problem `demo3` provides an example of this. Figure 3.14 shows output from the `convergence_table` command after running `eigenvalue_convergence` with a range of `nmesh2` values, for typical values of the control parameter and wave speed. The upper two convergence tables show the results obtained with `order`= 1 for eigenvalues 9 and 2, while the lower two tables show the



(a)



(b)

Figure 3.13: Eigenvalue spectra of periodic travelling wave solutions for the problem `demo3`. The control parameter values in (a) and (b) are such that the wave is stable and unstable, respectively. These figures illustrate that the onset of instability is associated with the spectrum crossing the imaginary axis away from the origin, i.e. it is of Hopf type. The dots indicate the (rather poor) approximations to eigenvalues corresponding to periodic eigenfunctions, calculated by discretising the eigenfunction equation, and the colours along the curves indicate the phase difference in the eigenfunction over one period of the periodic travelling wave. The run and plot commands used to generate these figures are given in the main text, and are also listed in the Appendix. The quantities eps, f and q referred to in the second line of the title are parameters which appear in the equations but which are not being used as the control parameter; their values are specified in the file `other_parameters.input` (see §2.2.3).

(a) `order=1`

nmesh	Re of evalue 9	Im of evalue 9	Error bound 9
100	-0.42201304E-01	0.24051920E+01	0.55334430E-04
200	-0.71010858E-01	0.86053281E+01	0.34546716E-05
400	-0.65037266E-01	0.87937590E+01	0.11489065E-04
800	-0.66672646E-01	0.88431720E+01	0.39065761E-04
1200	-0.67058826E-01	0.88524301E+01	0.11296455E-03

nmesh	Re of evalue 2	Im of evalue 2	Error bound 2
100	0.10474546E+00	0.49714409E+01	0.44593174E-04
200	0.24245619E-01	0.59628161E+01	0.12892151E-04
400	-0.81155430E-02	0.60342199E+01	0.83242802E-04
800	-0.12355648E-01	0.88670188E+00	0.18454233E-01
1200	-0.11838610E-01	0.88681645E+00	0.41529717E-01

(b) `order=2`

nmesh	Re of evalue 9	Im of evalue 9	Error bound 9
100	-0.85883103E-01	0.87211437E+01	0.22435235E-01
200	-0.68847449E-01	0.88493459E+01	0.25447809E-02
400	-0.67493922E-01	0.88591701E+01	0.22255001E-02
800	-0.67363382E-01	0.88598102E+01	0.16993811E-01
1200	-0.73503679E-01	0.17237650E+01	0.20880794E+02

nmesh	Re of evalue 2	Im of evalue 2	Error bound 2
100	-0.41847151E-02	0.00000000E+00	0.12590945E+00
200	-0.12490974E-01	0.88671728E+00	0.59945934E+00
400	-0.15447779E-01	0.88308056E+00	0.25714288E+01
800	-0.11372513E-01	0.88860381E+00	0.10258903E+02
1200	-0.22987593E-01	0.60612471E+01	0.10648373E+01

Figure 3.14: The change in the eigenvalues of the discretised eigenfunction equations as the constant `nmesh2` (defined in `constants.input`) is varied. In (a) the parameter `order` (also defined in `constants.input`) has been changed to 1; in (b) it has been reset to 2. The run command for these tables is `eigenvalue_convergence demo3 8.21E-4 9.75 100 200 400 800 1200` (the same for both (a) and (b); the only difference is the value of `order`). These commands are very time-consuming because of the large values of `nmesh2`: run times are about 15 hours for (a) and 20 hours for (b) on a typical desktop computer. Assuming that these are the first two runs of the `eigenvalue_convergence` command for `demo3`, they will be allocated ecode values of 101 and 102. The tables shown can then be generated via the commands `convergence_table demo3 101 9` and `convergence_table demo3 101 2` for (a), and `convergence_table demo3 102 9` and `convergence_table demo3 102 2` for (b).

corresponding results for order= 2. It is typical that as nmesh2 is increased, the error bounds on the eigenvalues increases, and there is a corresponding increase when order is increased for fixed nmesh2. Both of these trends are clear in Figure 3.14, for both of the eigenvalues. These trends occur because for the matrix arising from discretising the eigenfunction equation, the condition number increases as the discretisation becomes a better approximation to the eigenfunction equation, which has a zero eigenvalue. Considering first eigenvalue 9 for order= 1, the results in Figure 3.14 strongly suggest convergence to an eigenvalue of about $-0.067 + 8.8i$ as nmesh2 is increased. For order= 2, the eigenvalue approaches this value more rapidly as nmesh2 is increased, but then moves away as it becomes dominated by numerical error. For eigenvalue 2, the pattern is the same, but the error bounds are much more significant relative to the real part of the eigenvalue.

When choosing values for nmesh2 and order, it must be remembered that any inaccuracies in the eigenvalue approximations do not lead to inaccuracies in the computed spectrum – all that is required is that the approximations are sufficiently good that they converge to the points with $\gamma = 0$ on the computed spectrum. In the constants.input file for demo3, the settings nmesh2=400 and order = 2 are used as a compromise between accuracy and run time, and all of the 12 eigenvalues considered do converge to the points with $\gamma = 0$ on the computed spectrum, for all of the parameter sets considered. Here the number 12 is the value of nevalues, set in constants.input. Note that for publication or presentation purposes it would clearly be best to omit the dots showing the eigenvalues corresponding to periodic eigenfunctions in Figure 3.13, and this can be achieved by changing the plotter setting showperiodiceigenvalues to no in plot_defaults.input (see §3.4.1).

3.1.12 Multiple Simultaneous Runs of WAVETRAIN

The WAVETRAIN commands create and delete a number of temporary files during execution. Consequently it is not possible to run more than one command simultaneously, since these files might get deleted or overwritten in an inappropriate way. Such simultaneous runs are prevented by the creation of the file lockfile at the start of a command, which is deleted when the command finishes. Specifically, the following WAVETRAIN commands are protected via the creation of lockfile: add_points_list, add_points_loop, bifurcation_diagram, cleanup, eigenvalue_convergence, hopf_locus, new_pcode, period_contour, ptw, ptw_loop, stability, stability_boundary, stability_loop. Any other command can be used while one of these protected commands is being run. If a user wishes to run two of the protected WAVETRAIN commands in parallel, this is possible by installing two copies of WAVETRAIN in different parent directories. The two copies will be entirely decoupled, and plotting will then also have to be done separately in the two main directories.

In the same way, two simultaneous runs of the plot command are not possible because shell scripts are run in preparation for plotting that create various temporary files. Such simultaneous runs are prevented by the creation of the file plot_lockfile when the plot command is run; this file is deleted by the @quit or @exit commands.

However WAVETRAIN plotting can be done at the same time as new runs: there is no

conflict regarding temporary files. Note that although the WAVETRAIN plotter does of course use the `plot_defaults` and `.style` input files, it does not require any of the run input files, which can therefore be changed as desired between runs. Moreover, note that the output subdirectory for a WAVETRAIN run contains a copy of all of the run input files as they were when the command was run, providing a full record of the run (see §4.4 for details).

3.2 Details of `defaults.input`

This file is located in the main `input_files` directory, and contains the values of computational constants that the user will only rarely want to change. This file complements the `constants.input` files in subdirectories of `input_files`, which contain the constants that are expected to vary between problems. Apart from comment lines, the version of the file provided at installation is as follows.

```
 0.00001 0.001 # controlatol controlrtol
 0.00001 0.001 # speedatol speedrtol
 0.1 0.05 # periodatol periodrtol
 9999 9999 500 9999 9999 10 # nmx:  hb, ptw, bd, spectrum, sb, dummy
 0.0 100.0 # a0 a1
 1.0E-6 1.0E-6 1.0E-4 # epsl epsu epss for Hopf bifn & ptw continuation
 1.0E-5 1.0E-5 1.0E-3 # epsl epsu epss for spectrum & stability bdy
 0.0001 -1 # evzero evibound
 0.1 # gextra: overlap between plotted segments of the spectrum
 1 # help display (1/2=scroll/list)
 1.0E-8 # tolss: rel error tol on ptw variables for num soln of st st
 200 300 # nwarn1 nwarn2: thresholds for warnings about number of steps
 0.5 # grange: phase diff interval over which to search for fold
 0.001 # gatol: abs tol for phase diff, used only for Hopf stab bdy
 f77 # fortran77 compiler, can include option flags
    # blas:  blank, or name of user version (incl full path)
 y # lsame:  y/n = use/do not use the wavetrain version
    # dlamch:  blank, or name of user version (incl full path)
```

The meaning of the various constants is as follows.

`controlatol, controlrtol`

: After the continuation of the periodic travelling wave solutions finishes, the tolerances `controlatol` and `controlrtol` are used to assess whether the required value of the control parameter has been reached. The criterion is that the absolute value of (`control_parameter_soln`−`control_parameter_target`) be less than abs(`controlatol`)+abs(`controlrtol`∗`control_parameter_target`). These tolerances are needed because in AUTO a successful solution output at the specified value of the control parameter will not (necessarily) be exactly at the target value: AUTO has its own tolerance, which is determined by `epss`. However it is not feasible for WAVETRAIN to use the same tolerance criterion as AUTO because the AUTO criterion is based on continuation arc length. If the target value of the control parameter is assessed as not having been reached when in reality AUTO has reached it successfully, then either `controlatol` and/or `controlrtol` should be made smaller,

or epss (for ptw continuation) should be made larger.

speedatol, speedrtol
: The tolerances speedatol and speedrtol are analogous to controlatol and controlrtol, but for the wave speed. When calculating Hopf bifurcation loci and period contours, continuation is sometimes done using the wave speed as the main continuation parameter. In such cases, the tolerances speedatol and speedrtol are used to assess whether the end points of the continuation range have been reached, via the criterion that abs(speed−speed_end) must be less than the critical value abs(speedatol)+abs(speedrtol∗speed_end) in order for the end value speed_end to be assessed as having been reached. These tolerances are needed because in AUTO a successful solution output at the specified value of the wave speed will not (necessarily) be exactly at the target value: AUTO has its own tolerance, which is determined by epss. However it is not feasible for WAVETRAIN to use the same tolerance criterion as AUTO because the AUTO criterion is based on continuation arc length. If the target value of the wave speed is assessed as not having been reached when in reality AUTO has reached it successfully, then either speedatol and/or speedrtol should be made smaller, or epss (for ptw continuation) should be made larger.

periodatol, periodrtol
: One of the methods of calculating period contours involves specifying the required period. In this case, the tolerances periodatol and periodrtol are used to assess whether the required period has been reached. The criterion is that the absolute value of (period−period_target) be less than abs(periodatol)+abs(periodrtol∗period_target). These tolerances are needed because in AUTO a successful solution output at the specified value of period will not (necessarily) be exactly at period_target: AUTO has its own tolerance, which is determined by epss. However it is not feasible for WAVETRAIN to use the same tolerance criterion as AUTO because the AUTO criterion is based on continuation arc length. If WAVETRAIN assesses that the target value of period has not been reached when in reality AUTO has reached it successfully, then either periodatol and/or periodrtol should be made smaller, or epss (for ptw continuation) should be made larger.

nmx
: The nmx values specify the maximum number of continuation steps used in the various numerical continuation calculations.

  nmx_hb is used when locating the Hopf bifurcation in the periodic travelling wave equations.

  nmx_ptw is used for continuation of branches of periodic travelling wave solutions, except in bifurcation diagram calculations. It is used in the calculation of contours of constant period. It is also used for tracing the locus of Hopf bifurcation points in the control parameter–wave speed plane (though the starting point on this locus is found using nmx_hb).

`nmx_bd` is used for the continuation of branches of periodic travelling wave solutions in bifurcation diagrams.

`nmx_spectrum` is used for continuation along the eigenvalue spectrum.

`nmx_sb` is used for locating and continuing stability boundaries of both Eckhaus and Hopf type.

`nmx_dummy` is used for all continuations in dummy parameters. Such continuations occur as an initial step in the calculation of the eigenvalue spectrum and of stability boundaries and in order to determine a starting solution for derivatives of the eigenfunction. In the calculations of stability boundaries and of periodic travelling waves when using an indirect search method, there are some short continuations used to test the continuation direction, and `nmx_dummy` is also used for these.

For dummy parameter continuations, the `nmx` value will determine the end point of the continuation and a small value is recommended; however `nmx_dummy` should not be too small because of its use in the assessment of continuation directions; the recommended value is 10. For `nmx_hb`, `nmx_ptw` and `nmx_spectrum`, the setting should be large enough that computations do not end because the number of steps reaches `nmx`, except perhaps in the case of an error in the values of `ds`, `dsmin` or `dsmax` (given in `constants.input`). The recommended settings are 9999, simply because AUTO output (which appears in the `info.txt` file, and on the screen if the constant `info` is set to 4) can be confusing when step numbers have more than four digits: the values can be increased above 9999 should this prove necessary.

The constant `nmx_bd` should typically not be set to such a large number. Bifurcation diagram continuations stop because either limits on the continuation parameter (which is either the control parameter or the wave speed) or on the solution amplitude are exceeded, or because the maximum number of continuation steps is reached, or because of a convergence error (which often indicates that a homoclinic solution is being approached). This contrasts with other continuations done in WAVETRAIN, for which there is one or more target values of the continuation parameter at which the continuation ends. The appropriate value should be large enough to allow the solution branch to approach the homoclinic solution when this is the end point, but small enough that the run time is not excessive if there is some other end point (for example the solution branch might ping-pong between two different Hopf bifurcations, in which case AUTO will typically compute backwards and forwards repeatedly along the same solution branch).

`a0, a1`

The constants `a0` and `a1` are the lower and upper limits on the solution amplitude: continuation will stop if this is exceeded. The same values are used in all AUTO runs. Suitably small and large values respectively are recommended: it is not expected that continuation will ever stop because these limits are reached, during normal execution. Note that the L2-norm is used for the solution amplitude in all AUTO runs (this corresponds to setting the AUTO parameter `iplt` to 0).

`epsl, epsu, epss`

The constants `epsl`, `epsu` and `epss` are tolerance parameters for convergence criteria during AUTO runs. The constants are exactly as used in AUTO: `epsl` and `epsu` determine the relative convergence criteria for equation parameters and solution components respectively, in the Newton/Chord method used by AUTO, while `epss` determines the relative convergence criterion for the detection of special solutions. The recommended ranges are 10^{-6} to 10^{-7} for `epsl` and `epsu`, and 10^{-4} to 10^{-5} for `epss`. (In particular, `epss` should be 100 to 1000 times larger than `epsl` and `epsu`). The first trio of values is used for locating Hopf bifurcations, for continuing branches of periodic solutions, and for calculating contours of constant period, bifurcation diagrams, and Hopf bifurcation loci. The second trio of values is used for spectrum continuations and for the calculation of stability boundaries of both Eckhaus and Hopf type. To speed up execution it is recommended that the second trio is larger than the first.

`evzero`

The constant `evzero` is used by the commands `stability` and `stability_loop`. These commands calculate the spectrum, and then loop round the points in the calculated spectrum, looking for folds. The periodic travelling wave is assessed as being unstable/stable according to whether there is/is not a fold away from the origin in the right hand half of the complex plane. The constant `evzero` is used to assess whether a fold is "away from the origin": the criterion is that the amplitude of the fold location is greater than `evzero`. The constant `evzero` is also used by the `stability_boundary` command, which locates the fold away from the origin with largest real part as a precursor to detecting changes in stability of Hopf type.

`evibound`

The first stage in the calculation of the spectrum involves discretising the eigenfunction equation in the travelling wave coordinate, with periodic boundary conditions, and solving the resulting matrix eigenvalue problem. The matrix eigenvalues are ordered by the size of their real part, and a number `nevals` of them are used as starting points for continuation of the spectrum, with the constant `iposre` determining whether or not to include eigenvalues whose imaginary part is strictly negative; `nevals` and `iposre` are specified in `constants.input`. In some cases it is convenient to exclude from consideration matrix eigenvalues whose imaginary part exceeds a particular threshold in absolute value, and the constant `evibound` specifies this threshold. If `evibound` is negative, then no threshold is applied.

`gextra`

Let γ denote the phase difference in the eigenfunction across one period of the periodic travelling wave. Then the constant `gextra` determines the range of values of γ for which each spectrum segment is calculated: the range is $0 < \gamma < 2\pi + $ `gextra`. This entire range is plotted by the plotter command `@spectrum`. There is no problem with setting `gextra` to zero, but a small non-zero value of `gextra` may help the visual appearance of the spectra, by preventing gaps between successive segments. Also, it might occasionally be useful to set `gextra` to a much larger value as a diagnostic

tool. To ensure that $\gamma = 2\pi$ and $\gamma = 2\pi +$ `gextra` can be resolved as separate output points during continuation, `gextra` is interpreted as zero if it is less than 10∗`dsmin`.

`help display`
: Output from the `wt_help` command can be displayed by either scrolling or listing the help file. The code number determines which of these display formats is used. Scrolling is accomplished via the `man` facility on the user's system. Note that the help display format for the plotter's `@help` command is set separately, in `plot_defaults.input`.

`tolss`
: In general, there will not be an exact formula for the steady state, and therefore this will have to be found numerically, using the user-supplied formulae/values as an initial guess. This numerical solution is done using the minpack routine `hybrd1` (Moré *et al*, 1984), which uses a modification of the Powell hybrid method, and which is freely available from `www.netlib.org`. This routine gives a solution for which the estimated relative error in the solution is at most `tolss`.

`nwarn1, nwarn2`
: Very large or very small numbers of continuation steps are not desirable at any stage of the calculation. A large number of steps typically means long run times, possibly unnecessarily. A small number of steps means that bifurcation points might be jumped over without detection. WAVETRAIN gives a warning message if the number of steps in any stage of the calculation is either very small or very large. The constants `nwarn1` and `nwarn2` (`nwarn1` $<$ `nwarn2`) are the thresholds for these warning messages to be given.

`grange`
: When the change in periodic travelling wave stability is of Hopf (rather than Eckhaus) type, the first step in locating and tracking the stability boundary is to locate the point in the spectrum, away from the origin, at which there is a fold with the largest real part. This is calculated approximately when calculating the spectrum, in order to assess wave stability, but in order to calculate the stability boundary precisely a more accurate calculation must be done, via continuation of the equations for the first derivative of the eigenfunction (with respect to $i\gamma$) as well as the eigenfunction; here, as above, γ denotes the phase difference in the eigenfunction across one period of the periodic travelling wave. This can be a time-consuming calculation and therefore it is helpful to reduce the range of $i\gamma$ values over which it must be done. The constant `grange` specifies this range: if γ_{max} is the estimated fold location based on the spectrum calculation, then the range of γ values used to search for the exact location of the fold is $\gamma_{max} -$ `grange`$/2 < \gamma < \gamma_{max} +$ `grange`$/2$.

`gatol`
: With γ, `grange` and `gmax` as described above, a preliminary stage in the calculation of a stability boundary of Hopf type is to continue the spectrum up to the point with $\gamma =$ `gmax` $+$ `grange`$/2$. The tolerance `gatol` is used to assess whether this end

value of γ has been reached. Since it is known that γ takes values between roughly 0 and 2π, a single (absolute) tolerance is sufficient, and a relative tolerance is not required. Note that it is essential that `gatol` is significantly smaller than `grange`. If WAVETRAIN assesses that the target value of γ (which is `gmax`+`grange`/2) has not been reached when in reality AUTO has reached it successfully, then either `gatol` should be made smaller, or `epss` (for spectrum continuation) should be made larger.

`fortran77 compiler`

This is the name of the Fortran77 compiler to be used, e.g. `f77` or `g77`. It can be followed by one or more option flags. One reason for including a user-specified flag would be if by default the compiler outputs a list of subroutines during compilation. While this would not cause any errors for WAVETRAIN, it does interfere significantly with screen output and therefore should be suppressed. The appropriate flag for this is compiler dependent, but `-silent` or `-fsilent` are likely possibilities. Note that the "`-`" symbol does need to be specified (e.g. `f77 -fsilent`).

`blas`

BLAS (Basic Linear Algebra Subprograms) are used extensively by LAPACK; in WAVETRAIN, LAPACK is used to calculate approximations to the eigenvalues and eigenfunctions for the case when the eigenfunctions are periodic over one period of the periodic travelling wave. WAVETRAIN is supplied with the Fortran77 reference implementation of the BLAS (specifically the BLAS files that are distributed with version 3.1.1 of LAPACK), and this will usually be adequate. However calculations done by LAPACK are significantly faster if one uses a machine-specific optimised BLAS library. Such libraries are freely available for many computer architectures: see `www.netlib.org/blas` for details. This entry in `defaults.input` provides the user with the opportunity to use such a machine-specific library, by giving the file name including full path. The file name can be either an uncompiled fortran (`.f`) file, or a compiled (`.o`) file, or a library (`.a`). In the third case, the entry must also include the library path, e.g. `-L/usr/lib -lmyblas` (for the library `/usr/lib/libmyblas.a`). Note that whatever the user enters on this line of `defaults.input` is used directly in the Fortran77 compilation command for the eigenvalue calculation program. Alternatively the entry can be blank, in which case WAVETRAIN will use the Fortran77 reference implementation of the BLAS. Typically the calculations done by LAPACK constitute only a relatively small part of the run times in WAVETRAIN and therefore it is recommended that the Fortran77 reference implementation of the BLAS be used unless the user already has a machine-specific optimised BLAS library.

`lsame`

The Fortran77 function `LSAME` is used by both BLAS and LAPACK. If the user is providing their own version of BLAS (see above) then this may or may not include the function `LSAME`. If it does then the version of `LSAME` supplied with WAVETRAIN should be excluded from compilation of the eigenvalue calculation program, by entering `n` in this line of defaults.input. If the user-supplied BLAS does not include `LSAME`, or if the Fortran77 reference implementation of the BLAS is being used, then `y` should be entered on this line, to indicate that the version of `LSAME` supplied with WAVETRAIN

should be included in the compilation.

`dlamch`
: The Fortran77 function `DLAMCH` is used by LAPACK, and returns the value of "machine epsilon", which gives a bound on the roundoff in individual floating-point operations. A version of this function is distributed with LAPACK (version 3.1.1), and this is supplied with WAVETRAIN. This function will work on the vast majority of computers, but not all. In the latter case, the user can enter on this line of defaults.input the name (including full path) of a file containing an alternative version of `DLAMCH`. The file can be either an uncompiled (`.f`), or compiled (`.o`) file, or a library (`.a`) containing the function. In the third case, the entry must also include the library path, e.g. `-L/usr/lib -lmylibrary` (for the library `/usr/lib/libmylibrary.a`). Note that whatever the user enters on this line of defaults.input is used directly in the Fortran77 compilation command for the eigenvalue calculation program. If the entry is blank, then the version of `DLAMCH` supplied with WAVETRAIN will be used.

3.3 Further Details of Plot Commands

3.3.1 Changing Plotter Styles

One of the objectives of WAVETRAIN is to produce graphical output suitable for publication. In many cases, users will wish to produce greyscale plots for this purpose, although during the research process they may find it more convenient to use colours to distinguish the different line and point types. To switch to greyscale mode, one enters the plot command

```
@set_style greyscale
```

and one can type

```
@set_style colour
```

to return to colour output. Note that the `@set_style` command creates a new postscript file of the parameter plane key, such as that illustrated in Figure 2.4 on page 19. Therefore if a postscript file is being written then it is ended by the `@set_style` command, with plotting returned to the screen after the command finishes.

Users may also wish to create their own plotter styles. To do this, one goes into the `input_files` directory and copies either `colour.style` or `greyscale.style` to a new file such as `my_settings.style`. The various settings in this file are discussed in §3.4; they cover the colour, thickness and style of all lines, plus point colours and types. The explanatory information in §3.4.2 is repeated in comments in the versions of `colour.style` and `greyscale.style` provided at installation; these comments describe in detail the meaning of each setting. The available line styles are explained in these comments. For colours, a total of 186 colours are available in WAVETRAIN, consisting of the 133 standard Crayola crayon colours, colours of the rainbow, primary and secondary colours (which are not all

standard Crayola crayon colours), and 50 shades of grey, named grey1 (almost black) up to grey50 (almost white). A list of these colour names is provided as `colour_list.eps` in the `postscript_files` directory; this list is reproduced in Figure 3.15. Note that `colour_list.eps` is recreated each time the plotter is started. For details of Crayola crayon colours, see `http://en.wikipedia.org/wiki/List_of_Crayola_crayon_colors`.

3.3.2 Changing Other Plotter Settings

A variety of other plotter settings are contained in the file `plot_defaults.input` in the `input_files` directory. This includes the choice of plotter (`sm` or `gnuplot`), the specification of font sizes for text, the line and column spacings in the keys, the default choice of plotter style file, and the default choice between code numbers, symbols and wave period in parameter plane plots. These and other settings can all be changed by the user if desired, by editting `plot_defaults.input`, which contains detailed comments explaining the meaning of each setting. The settings are also explained in detail in §3.4. After editting `plot_defaults.input`, the plotter must be restarted in order for the changes to take effect.

3.3.3 Labelling of Contours of Constant Period

If `showperiodcontourlabels` is set to `yes` in `plot_defaults.input`, then the plot command `@period_contour` draws the specified contour(s) and also annotates it/them with labels showing the value of the period. By default, these labels are placed where (and if) a contour crosses the edge of the plotting region. This is appropriate in some cases, but in others it does not give clear labels. Therefore the plot command `period_contour` provides the opportunity to override this default. When prompted, the user can enter one or more expressions of the form <control_parameter_name> = <value> or <wave_speed_name> = <value>. This causes the default labels to be omitted, and instead labels are placed wherever (and if) a contour crosses the specified values.

As an example, consider the plot shown in Figure 2.5 on page 22, which used default labelling for the two period contours. Instead, for the plot command

```
@period_contour 101
```

one could enter

```
c=0.8 c=0.5
```

when prompted about label locations. Similarly, for the plot command

```
@period_contour 102
```

one could enter

```
c=0.7 A=0.5 A=0.8 c=0.4
```

when prompted about label locations. (Note that pcodes 101 and 102 refer to the contours with periods 3000 and 80 respectively). The resulting plot is shown in Figure 3.16. Note that the label specification "`A=0.8`" for pcode 102 has no effect, since the contour does not cross this value.

Figure 3.15: A list of the colours available in the WAVETRAIN plotter. This figure is a reproduction of the file `colour_list.eps` in the `postscript_files` directory. The US spelling "gray" may be used as an alternative to the UK spelling in any colour name: thus "gray23" and "bluegray" are permitted. Note that the Crayola crayon colour names "gray" and "tan" have been replaced by "crayolagray" (or "crayolagrey") and "crayolatan" respectively. In the first case this avoids any confusion with the grey scale colour names; in the second case it avoids confusion with the mathematical function tan.

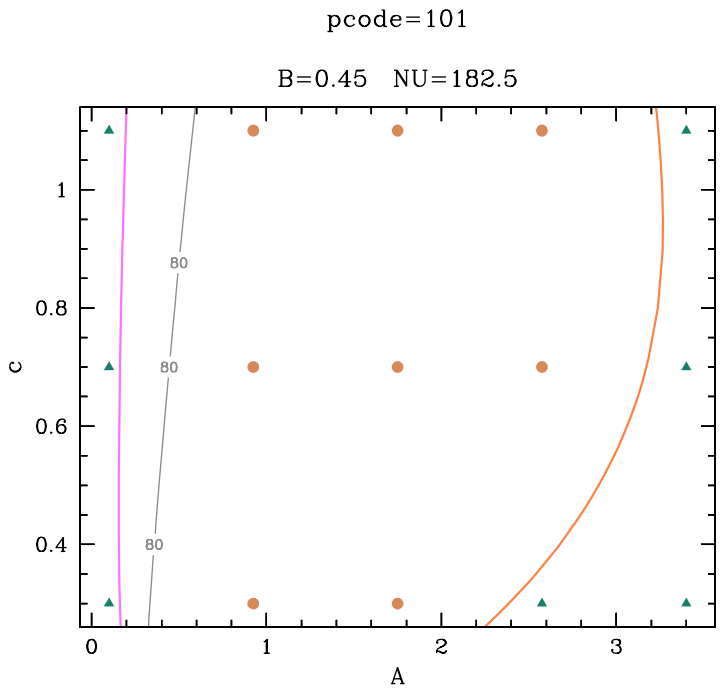


Figure 3.16: An illustration of manual specification of the label locations for contours of constant wave period. This figure is the same as Figure 2.5 except that in this case the default label locations for the contours have been overridden. The run and plot commands used to generate this figure are given in the main text, and are also listed in the Appendix.

3.3.4 Adding Additional Lines, Points and Text to Plots

The plot command

`@line` x_1 y_1 x_2 y_2

superimposes a line between (x_1,y_1) and (x_2,y_2) in the current plot. Similarly,

```
@point x y
```

draws a point (symbol) at (x,y); the symbol type is specified in the `.style` file. For text labels, the command

```
@text x y "my text"
```

writes "my text" centred at the point (x,y). For all three commands, coordinates can be enclosed in double quotes. In `sm` this is optional, but in `gnuplot` it is essential if the coordinates are negative. Thus `@point -1.0 2.0` is invalid in `gnuplot` and gives an error; instead one must use `@point "-1.0" 2.0` or equivalently `@point "-1.0" "2.0"`.

As an example of the use of these commands, consider the bifurcation diagram plot in Figure 3.2b on page 78. This plot gives a detailed account of the existence of periodic travelling wave solutions as the wave speed c is varied for control parameter $A = 2.6$. However, it contains no information about stability, and indeed WAVETRAIN does not have the facility to compute stability in a bifurcation diagram. However, one can determine where the stability boundary curve crosses the line $A = 2.6$ via an optional argument to `stability_boundary`, for instance

```
stability_boundary demo 102 1.75 0.3 1.75 0.7 A=2.6
```

where 102 is an appropriate pcode value. This run reports that there is a change in wave stability at $A = 2.6$, $c = 0.66$. One can then add this information to the bifurcation diagram plot by typing

```
@line 0.66 10.0 0.66 20.5
```

at the plotter prompt, after drawing the bifurcation diagram. One might also wish to add labels indicating which part of the solution branch is stable via

```
@text 0.5 13.5 "Unstable"
```

and the command `@text 0.9 13.5 "Stable"` might be used in a similar way. The resulting plot is illustrated in Figure 3.17.

There are two other related plot commands: `@linesfile` and `@pointsfile`. These both plot data supplied by the user and contained in a file in the relevant input subdirectory; the file name is entered as a command argument. The file must contain two columns of numerical data, which are a set of coordinates to be plotted; other columns are allowed in the file and will be ignored. Thus

```
@linesfile myfile.dat
```

will draw lines connecting the various points whose coordinates are in the first two columns of `myfile.dat` in the relevant input subdirectory. The command `@pointsfile` has a second argument, specifying the point type to be used, according to the code numbers listed on page 127. Thus

```
@pointsfile myfile.dat 9
```

will draw a filled triangle at each of the points whose coordinates are in the first two columns of `myfile.dat` in the relevant input subdirectory. One potential use of the commands `@linesfile` and `@pointsfile` is to superimpose onto WAVETRAIN plots results from numerical simulations of the partial differential equations; an example of this is given in §2.3.25.

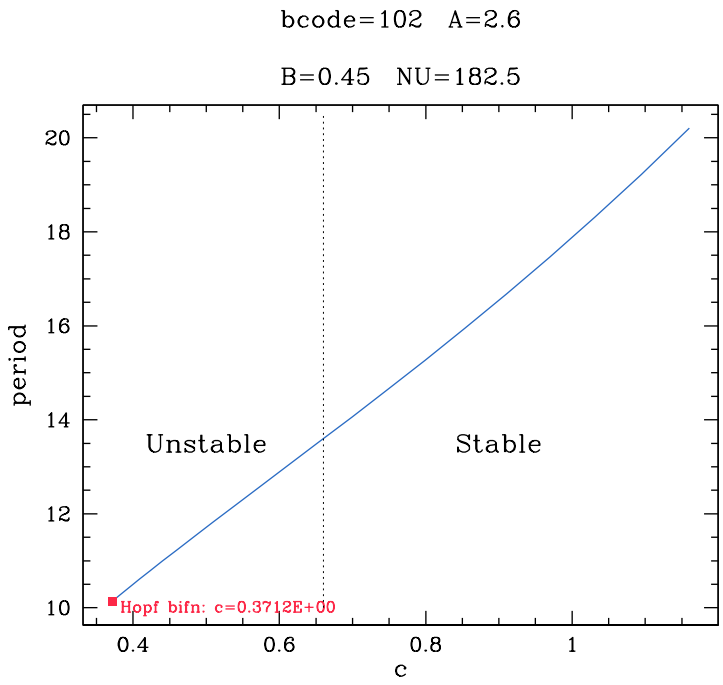


Figure 3.17: An illustration of the use of the plot commands `@line` and `@text`. These commands have been used to indicate the change in wave stability on a bifurcation diagram for the problem `demo`. The run and plot commands used to generate this figure are given in the main text, and are also listed in the Appendix.

3.3.5 Record Keeping for Postscript Plots

When generating postscript plots for publication or presentation, users may wish to retain a record that would enable them to recreate the plot at a later date. This can be achieved by setting the plotter variable `keeprecords` to `yes` in `plot_defaults.input`. This setting causes the `@postscript` command to generate a plotting record as well as the postscript file. For example, the command `@postscript demoplot` creates the directory `demoplot_record` which contains two files. The first of these, `demoplot.tar`, is an archive of all of the data used for `demoplot.eps`; the second file, `demoplot.plt`, is a list of the various plot commands and option choices used to generate the plot, plus a listing of the plotter input files (see §3.4). Together these provide a full record that would enable the plot to be reproduced from scratch. This record-keeping facility should be used with care, simply because the `.tar` record files can be rather large. For this reason, the default setting of `keeprecords` is `no`.

3.3.6 Abbreviations for Plot Commands

Typically, users will want to enter plot commands repeatedly in relatively rapid succession, making the full command names rather cumbersome. Therefore, the plotter also recognises a number of two-letter shorthands:

```
@bd  =  @bifurcation_diagram
@hl  =  @hopf_locus
@pc  =  @period_contour
@pp  =  @pplane
@ps  =  @postscript
@sb  =  @stability_boundary
@sp  =  @spectrum.
```

3.4 Details of Plotter Input Files

3.4.1 Details of `plot_defaults.input`

This file contains general default settings associated with plotting; the order of the various entries in the file does not matter. Settings concerning colours, line thicknesses and line styles are in the `.style` files, described in §3.4.2. The version of the file provided at installation contains detailed comments explaining the meaning of each setting. Note that if plotting is being done using `gnuplot`, then text size settings will only take effect if enhanced text mode is specified in the terminal setting. (The terminal setting is specified in this file, as part of the plotter setting `plotter`).

3.4.1.1 General default settings

`colourlistexpand` (setting at installation: `0.8`)
: This determines the font size for the list of colours created (in a postscript file) by the command `@set_colours`.

`defaultstyle` (setting at installation: `colour`)
: This determines the default style file that will be set when the plotter is started. The plotter style can be changed using the command `@set_style`.

`keeprecords` (setting at installation: `no`)
: If this is set to `yes` then when a a postscript file is generated, a record is created of all of the run and plotter commands that were used to generated the plot. The record consists of two files, which have the names `file.tar` and `file.plt`, where `file.eps` is the name of the postscript file. These files are both placed in a subdirectory `file_record` of the directory containing `file.eps` (which is itself a subdirectory of `postscript_files`). One of these files, `file.tar`, is an archive of all of the output data files for the subdirectory and pcode value given in the `plot` command. Note that these output files contain a copy of all of the input data files used in the run commands. The other record file, `file.plt`, is a list of the plot commands used to create the plot, followed by a listing of `plot_defaults.input`, as it was when the plot command was given, followed by a listing of the style file (e.g. `colour.style`)

that applied when the postscript file was generated. Taken together, these two record files contain all of the information that would be required to regenerate the plot from scratch. Setting `keeprecords` to `no` disables this record-keeping feature.

`labelsexpand` (setting at installation: `1.5`)
: This determines the font size for axes labels.

`plotter` (setting at installation: `gnuplot wxt 0 enhanced font "Sans,10"`)
: This is the name of the plotter to be used, in lower case: either `sm` or `gnuplot`. For `sm`, the plotting device is taken from the user's `.sm` file. For `gnuplot`, the terminal (for screen plots) must be specified after the word `gnuplot`, including options. Note that enhanced text mode must be specified in order for text size settings to have effect: if the terminal details do not contain the word `enhanced`, then font size settings will be ignored, and all text will be plotted at the default size. Note also that the font, including default text size, can be set as part of the terminal description if required (see `gnuplot` documentation for details). Elsewhere in `plot_defaults.input`, the plotter setting `screenwidthchars` is defined (used for `gnuplot` only, not `sm`). This is the average number of characters that will span the full width of the plotting canvas. Therefore if the font type or size in the `gnuplot` terminal specification is changed, this plotter setting will need to be changed too.

`screenwidthchars` (setting at installation: `105`)
: This is used for `gnuplot` only, not `sm`. It gives the width of the entire plotting canvas, as a number of average (unscaled) character widths. This will depend on both the `gnuplot` terminal type and the (unscaled) font type and size, which are specified in this file, as part of the plotter setting `plotter`. At installation, the terminal `wxt` with font `Sans,10` is specified, for which the appropriate value of `screenwidthchars` is 105. Note that the specified value can be either an integer or a floating point number.

`showtitles` (setting at installation: `yes`)
: This determines whether or not titles (with parameter values etc) are shown above the plots.

`spacebottom` (setting at installation: `0.17`)
`spaceleft` (setting at installation: `0.15`)
`spaceright` (setting at installation: `0.02`)
`spacetopnotitles` (setting at installation: `0.02`)
`spacetoptitles` (setting at installation: `0.15`)
: These settings determine the amount of space around the graph(s), as a proportion of the overall plotting "canvas". Thus the graph(s) itself occupies a region whose width is a fraction (1-`spaceleft`-`spaceright`) of the canvas width, and whose height is a fraction (1-`spacebottom`-`spacetoptitles`) of the canvas height if `showtitles` is set to `yes`, and a fraction (1-`spacebottom`-`spacetopnotitles`) if `showtitles` is set to `no`. The space around the graph(s) contains tic mark labels, axes labels and (if selected) title(s). The size of this space does not scale with the text size selected for axes labels and titles, and therefore may need to be adjusted if these are altered significantly from the defaults.

`ticlabelsexpand` (setting at installation: `1.3`)
: This is used for `sm` only, not `gnuplot`. It determines the font size for tic mark labels. This is included because it is convenient in `sm` to be able to change all text sizes relative to the default font, since the procedure for changing the default font in `sm` lies outside WAVETRAIN and would affect other uses of `sm`. Note that changing `ticlabelsexpand` also changes the size of the tic marks. For `gnuplot`, tic mark labels use the default font, which can be changed in the terminal specification, given as part of the plotter setting `plotter` elsewhere in this file.

`titlesexpand` (setting at installation: `1.5`)
: This determines the font size for titles.

`helpdisplay` (setting at installation: `1`)
: This determines whether the output from the plotter command `@help` is displayed by scrolling (`helpdisplay`=1) or listing (`helpdisplay`=2) the help file.

3.4.1.2 Settings for plots of eigenvalue spectra

`foldsymbolsizesp` (setting at installation: `2.0`)
: This determines the size of the symbol used to indicate the location of the right-most non-zero turning point in the eigenvalue complex plane (if `showspectrumfold` is set to `yes`); this turning point is used to determine stability.

`foldtextspexpand` (setting at installation: `0.98`)
: This determines the size of the font used for the real part of the eigenvalue at the right-most non-zero turning point in the eigenvalue complex plane (if `showspectrumfold` is set to `yes`); this turning point is used in the determination of stability, and also as a starting point for the calculation of stability boundaries of Hopf type.

`periodiceigenvaluessize` (setting at installation: `1.2`)
: This determines the size of the symbols used to denote periodic eigenvalues (if `showperiodiceigenvalues` is set to `yes`) on spectrum plots.

`restrictphasedifference` (setting at installation: `no`)
: This determines whether all or only parts of the spectrum is plotted, corresponding to a particular range of values of the phase difference across one period of the wave. Normally this should be set to `no`, but occasionally `yes` is useful for diagnostic purposes. In that case, the plotter command spectrum asks for keyboard entry of the desired range of phase difference values.

`showperiodiceigenvalues` (setting at installation: `yes`)
: For plots of eigenvalue spectra, this determines whether or not to label the approximations to the eigenvalues for periodic eigenfunctions, found via discretisation.

`showspectrumfold` (setting at installation: `yes`)
: This determines whether or not there is a label showing the real part of the eigenvalue at the right-most non-zero turning point in the eigenvalue complex plane; this turning point is used to determine stability.

`spectrumkeyheight` (setting at installation: `6`)

If `spectrumcolour` is set to `rainbow` or `greyscale` or `grayscale`, a key is included in spectrum plots showing the mapping from the colours to the phase difference across the periodic travelling wave. The height of this key is determined by `spectrumkeyheight`. It is the key height as a percentage of the overall height of the main plot, the key and the space between them. Any value less than or equal to zero causes the key to be omitted.

`spectrumkeyspacing` (setting at installation: `3`)

If `spectrumcolour` is set to `rainbow` or `greyscale` or `grayscale`, a key is included in spectrum plots showing the mapping from the colours to the phase difference across the periodic travelling wave. In `sm`, `spectrumkeyspacing` specifies the spacing between this key and the main plot, as a percentage of the overall height of the main plot, the key and the space between them. In `gnuplot`, the role of `spectrumkeyspacing` is the same, but it does not have such a precise meaning: larger values give more space between the key and the main plot, but precise automated control is not possible since the size of the main plot is somewhat unpredictable. Note that in `gnuplot`, manual rescaling of the main plot may be needed to achieve the required size; the user is prompted for keyboard input concerning this rescaling. Note also that in `gnuplot`, a negative value of `spectrumkeyspacing` can be used to reduce the gap between the key and the main plot: there may be a gap even if `spectrumkeyspacing` is set to zero. A negative value is never appropriate in `sm`.

`spectrumkeytextexpand` (setting at installation: `1.7`)

This determines the font size used in the key.

3.4.1.3 Settings for control parameter – wave speed plots

`periodcontourlabelsdps` (setting at installation: `0`)

This specifies the number of decimal places used when labelling period contours. This applies whether `periodcontourlabelsstyle` is set to `e` or to `f`.

`periodcontourlabelsexpand` (setting at installation: `0.9`)

This determines the font size for the labels indicating the value of the period along contours of constant period for periodic travelling wave solutions. Note that if this is changed, then `xperiodcontourlabelbox` and `yperiodcontourlabelbox` will usually need to be changed also.

`periodcontourlabelsstyle` (setting at installation: `f`)

This takes the value `e` or `f`, meaning exponential or floating point respectively. For example, with `periodcontourlabelsdps` set to 3, a period of 34.5621 will appear as `34.562` if `periodcontourlablesstyle` is set to `f`, and as `0.346e+2` if `periodcontourlablesstyle` is set to `e`.

`pplanecodesexpand` (setting at installation: `0.9`)

This determines the font size of the text used to denote run outcomes if `pplanetype`

is set to `rcodes` (or equivalents), or to `period` (or `periods`), or if these settings are selected manually.

`pplanegap` (setting at installation: `0.06`)
: The axes limits in control parameter – wave speed plots are set wider than the limits in `parameter_range.input`, to allow for the size of the rcodes/periods/symbols used to indicate the solution outcomes. The amounts added to the axes ranges are a fraction `pplanegap` of the ranges in `parameter_range.input`. Note however that if the parameter plane was generated using the `new_pcode` command, then the limits in `parameter_range.input` are used and `pplanegap` is not used.

`pplanekeygaplength` (setting at installation: `2`)
: This determines the length of the gaps between line segments and text in the key, as a percentage of the overall width of the key. The value must be an integer.

`pplanekeylinelength` (setting at installation: `8`)
: This determines the length of the line segments in the key, as a percentage of the overall width of the key. The value must be an integer.

`pplanekeylineseparation` (setting at installation: `7`)
: This determines the spacing of the lines in the key. Note that this spacing is not scaled by the font size selected for the text in the key, which is determined by `pplanekeytextexpand`, which is also defined in this file. Therefore if `pplanekeytextexpand` is changed, it may also be necessary to change the value of `pplanekeylineseparation`, to avoid the text on different lines overlapping.

`pplanekeylist` (setting at installation: `"{ 1 5 2 3 4 11 12 13 14 15 }"`)
: Note the inverted commas and curly brackets, which are both essential. This setting specifies which dots and line segments are used in the key for the control parameter - wave speed parameter plane plots. It also determines the order in which the dots (corresponding to outcome codes) and line segments are placed in the key. Numbers 1-5 indicate dots corresponding to the outcome codes, whose meaning is as follows:

  1: Periodic travelling wave found, stability not requested. This is the outcome code when `ptw_loop` is run and a periodic travelling wave is found.

  2: Periodic travelling wave found, and the spectrum shows that it is stable.

  3: Periodic travelling wave found, and the spectrum shows that it is unstable.

  4: No periodic travelling wave was found, with continuation along the periodic travelling wave solution branch ending for some reason other than a convergence problem.

  5: No periodic travelling wave was found, with continuation along the periodic travelling wave solution branch ending due to a convergence problem.

  Two digit numbers indicate line segments as follows:

  11: Hopf bifurcation loci.

12: Period contour.

13: Homoclinic bifurcation loci.

14: Stability boundary (Eckhaus type).

15: Stability boundary (Hopf type).

Note that if `pplanekeytype` is set to 2, then 4 and 5 would produce the same entry in the key, and if the number 4 is included in the list, it is ignored.

`pplanekeysymbolssize` (setting at installation: `2.0`)
This determines the size of dots in the key.

`pplanekeytextexpand` (setting at installation: `1.15`)
This determines the font size used for text in the key. Note that the spacing of lines in the key is determined by `pplanekeylineseparation`, which is also defined in this file. This is not scaled by `pplanekeytextexpand`, and therefore if `pplanekeytextexpand` is changed, it may also be necessary to change the value of `pplanekeylineseparation`, to avoid the text on different lines overlapping.

`pplanekeytype` (setting at installation: `1`)
This takes the value 1 or 2, and affects both the key for control parameter–wave speed plots, and the plots themselves. If it is set to 1, then separate colours and symbol types are used for the cases of no periodic travelling wave being found with a convergence failure in the numerical continuation, and of no periodic travelling wave being found with convergence throughout the continuation. Correspondingly, separate entries (with explanatory text) appear in the key. If pplanekeytype is set to 2, then the same colour and symbol type are used for the two cases (specifically, the colour and symbol type allocated to the case of convergence failure). Correspondingly, only one entry appears in the key. It is anticipated that most users will set `pplanekeytype` to 1 during the research process, and to 2 when producing figures for presentation or publication.

`pplanesymbolssize` (setting at installation: `2.0`)
This determines the size of the symbols used to denote run outcomes if `pplanetype` is set to `symbol` (or equivalents), or to `period` (or `periods`), or if these settings are selected manually.

`pplanetype` (setting at installation: `rcode`)
Allowable settings are:

`dot/dots/symbol/symbols`
`code/codes/number/numbers/rcode/rcodes`
`period/periods`.

(Note that the `sm` command `dot` is disabled via `overload` when `plot` is run). This determines whether parameter plane plots use symbols, rcode numbers or the period of the periodic travelling wave to denote the points in the parameter plane at which waves have been calculated. This is a default setting, and the user is given the opportunity to override it via keyboard input when the command `@pplane` is run.

Typically symbols would be used for final (presentation/publication) plots. Using rcode numbers is helpful for subsequent plotting of wave forms or eigenvalue spectra; however it can can make the plots very busy. Periods are helpful prior to calculating period contours. When the setting is period/periods, a symbol is used for parameter values for which there is no periodic travelling wave. Note also that periods below 10^{-9} are shown as zero, while those above 10^{10} are shown as `inf`.

`showperiodcontourlabels` (setting at installation: `yes`)
: This determines whether contours of constant period are labelled with the period values.

`xperiodcontourlabelbox` (setting at installation: `0.04`)
`yperiodcontourlabelbox` (setting at installation: `0.02`)
: When labels are used for a period contour, the contours are not plotted in a rectangular region centred on the label location. The dimensions of this region are 2×(control parameter range)×`xperiodcontourlabelbox` and 2×(wave speed range)×`yperiodcontourlabelbox`. Note that these dimensions are unaffected by `periodcontourlabelsexpand` and therefore they must usually be changed if `periodcontourlabelsexpand` is changed.

3.4.1.4 Settings for bifurcation diagram plots

`bdkeygaplength` (setting at installation: `2`)
: This determines the length of the gaps between line segments and text in the key, as a percentage of the overall width of the key. The value must be an integer.

`bdkeyheight` (setting at installation: `6`)
: This determines the height of the key (if present). It is the key height *per line* of the key, as a percentage of the overall height of the main plot, the key, and the space between them. (Note that whether or not there is a key, and the number of lines in the key if there is one, both depend on which plotting options are selected).

`bdkeylinelength` (setting at installation: `8`)
: This determines the length of the line, as a percentage of the overall width of the key. The value must be an integer.

`bdkeyspacing` (setting at installation: `4`)
: This determines the spacing between the key and the main plot, as a percentage of the overall height of the main plot, the key and the space between them.

`bdkeytextexpand` (setting at installation: `0.9`)
: This determines the font size used in the key.

`foldsymbolsizebd` (setting at installation: `2.0`)
: This determines the size of the symbols used to indicate the Hopf bifurcation point and also, if `showbdlabels` is set to `yes`, folds and end points.

`foldtextbdexpand` (setting at installation: `0.98`)
: This determines the size of the font used to label the Hopf bifurcation point, folds and endpoints, if `showbdlabels` is set to `yes`.

`showbdlabels` (setting at installation: `yes`)
: This determines whether folds and end points are labelled with filled circles, and whether the values of the control parameter at folds, at end points, and at the Hopf bifurcation point are written on the plot. The Hopf bifurcation point is always indicated by a filled square, even if `showbdlabels` is set to `no`.

3.4.1.5 Settings for the `@line`, `@point` and `@text` commands

`extrapointsize` (setting at installation: `2.0`)
: This determines the size of symbols generated by the `@point` command.

`extratextexpand` (setting at installation: `1.6`)
: This determines the font size for text generated by the `@text` command. Note that this does not affect any other text (axes labels, titles etc).

3.4.2 Details of Plotter Style File

This file contains settings associated with the plot style (colours, line thicknesses and line styles); the order of the various entries in the file does not matter. At installation, two different style files are provided: `colour.style` and `greyscale.style`; both contain detailed comments explaining the meaning of the various settings. The following list gives the value of each setting in the installation version of `colour.style`, as an example of a typical value.

3.4.2.1 Colour Settings

The available colours are listed in the file `colour_list.eps` in the `postscript_files` directory. They are based on the standard list of Crayola crayon colours, supplemented by cyan, and by 50 shades of grey (with grey01 being almost black and grey50 being almost white). The US spelling "gray" may be used as an alternative to the UK spelling in any colour name: thus "gray23" and "bluegray" are permitted. Note that the Crayola crayon colour names "gray" and "tan" have been replaced by "crayolagray" (or "crayolagrey") and "crayolatan" respectively. In the first case this avoids any confusion with the grey scale colour names; in the second case it avoids confusion with the mathematical function tan.

3.4.2.1.1 Colour settings for drawing periodic travelling wave solutions

`wavecolour` (setting in `colour.style`: `denim`)
: This specifies the colour used for drawing wave solutions, via `@ptw`.

3.4.2.1.2 Colour settings for plots of eigenvalue spectra

`spectrumcolour` (setting in `colour.style`: `rainbow`)

This specifies the colour used for drawing eigenvalue spectra. Any defined colour is allowed, or `rainbow`, or `greyscale` or `grayscale`. These three settings cause the spectrum to be coloured according to the phase difference in the eigenfunction over one period of the periodic travelling wave, using either a rainbow or greyscale colour map. An additional permitted setting is `none`, in which case the spectrum is not drawn; this enables plotting of just the eigenvalues corresponding to periodic eigenfunctions. Important note: in `gnuplot`, if variable colouring is requested via `spectrumcolour`="`rainbow`" or "`greyscale`" or "`grayscale`", the size of the main plot is somewhat unpredictable, and manual rescaling may be needed to achieve the required size; the user is prompted for keyboard input concerning this rescaling. Also, these settings cause ticmarks to be absent in `gnuplot`; ticmark labels are present, however. If desired, ticmarks could be added manually using the `@line` command.

3.4.2.1.3 Colour settings for control parameter – wave speed plots

`colour1` (setting in `colour.style`: `rawsienna`)
`colour2` (setting in `colour.style`: `orangered`)
`colour3` (setting in `colour.style`: `midnightblue`)
`colour4` (setting in `colour.style`: `vividviolet`)
`colour5` (setting in `colour.style`: `tropicalrainforest`)

These settings define the colours used in plots of the control parameter – wave speed plane, to indicate different outcomes. The same colour can be used for several outcomes, if desired.

1: Periodic travelling wave found, stability not requested. This is the outcome code when `ptw_loop` is run and a periodic travelling wave is found.

2: Periodic travelling wave found, and the spectrum shows that it is stable.

3: Periodic travelling wave found, and the spectrum shows that it is unstable.

4: If `pplanekeytype`=1, then this indicates that no periodic travelling wave was found, with continuation along the periodic travelling wave solution branch ending for some reason other than a convergence problem. If `pplanekeytype`=2, then this is not used.

5: If `pplanekeytype`=1, then this indicates that no periodic travelling wave was found, with continuation along the periodic travelling wave solution branch ending due to a convergence problem. If `pplanekeytype`=2, then this indicates simply that no periodic travelling wave was found.

`homocliniccolour` (setting in `colour.style`: `pinkflamingo`)

This specifies the colour used for the loci of homoclinic solutions (which are actually contours of waves of large period that have been designated as homoclinic).

`hopflocuscolour` (setting in `colour.style`: `mangotango`)

This specifies the colour used for the loci of Hopf bifurcations in the travelling wave equations.

`periodcontourcolour` (setting in `colour.style`: `grey28`)
: This specifies the colour used for contours along which periodic travelling waves have constant period.

`sbdyeckhauscolour` (setting in `colour.style`: `green`)
: This specifies the colour used for curve(s) indicating the boundary between stable and unstable waves, when the change of stability is of Eckhaus type.

`sbdyhopfcolour` (setting in `colour.style`: `violetblue`)
: This specifies the colour used for curve(s) indicating the boundary between stable and unstable waves, when the change of stability is of Hopf type.

3.4.2.1.4 Colour settings for bifurcation diagram plots

`bdlabelscolour` (setting in `colour.style`: `scarlet`)
: This specifies the colour used for text and symbols labelling folds, end points and the Hopf bifurcation point in bifurcation diagram plots.

`bdlinecolourmax` (setting in `colour.style`: `denim`)
`bdlinecolourmean` (setting in `colour.style`: `cerise`)
`bdlinecolourmin` (setting in `colour.style`: `denim`)
`bdlinecolournorm` (setting in `colour.style`: `junglegreen`)
`bdlinecolourperiod` (setting in `colour.style`: `denim`)
`bdlinecolourstst` (setting in `colour.style`: `turquoiseblue`)
: These settings specify the colours used for drawing the various properties of the periodic travelling wave solution branch.

3.4.2.1.5 Colour settings for the `@line`, `@point` and `@text` commands

`extralinecolour` (setting in `colour.style`: `black`)
: This specifies the colour of lines generated by the `@line` command. Note that this does not affect any other lines.

`extrapointcolour` (setting in `colour.style`: `black`)
: This specifies the colour of points generated by the `@point` command. Note that this does not affect any other symbols.

`extratextcolour` (setting in `colour.style`: `black`)
: This specifies the colour of text generated by the `@text` command. Note that this does not affect any other text (axes labels, titles etc).

3.4.2.2 Point Type Settings

The meaning of these settings is the same for `sm` and for `gnuplot` with `x11`, `wxt` or `postscript` terminals, except where noted below. However the meaning within `gnuplot` is terminal dependent, and if a different screen terminal is specified in `plot_defaults.input`, then the meanings may be different: this can be checked via `gnuplot`'s `test` command (see `gnuplot` documentation for details).

1: horizontal-vertical cross (like a + sign)

2: diagonal cross (like a "times" sign)

3: a star (like an asterisk sign)

4: open square

5: filled square

6: open circle

7: filled circle

8: open triangle

9: filled triangle

10: open upside-down triangle (like a "nabla" sign)

11: filled upside-down triangle (like a "nabla" sign)

12: open diamond (`gnuplot`)/filled hexagon (`sm`)

13: filled diamond (`gnuplot`)/filled hexagon (`sm`).

3.4.2.2.1 Point type settings for control parameter – wave speed plots

`pointtype1` (setting in `colour.style`: `7`)
`pointtype2` (setting in `colour.style`: `7`)
`pointtype3` (setting in `colour.style`: `7`)
`pointtype4` (setting in `colour.style`: `5`)
`pointtype5` (setting in `colour.style`: `9`)

These five settings refer to the five possible run outcomes, as for the settings `colour1`,...,`colour5`.

3.4.2.2.2 Point type settings for the `@line`, `@point` and `@text` commands

`extrapointtype` (setting in `colour.style`: `7`)

This setting is for symbols drawn with the `@point` command.

3.4.2.3 Line Thickness Settings

In these settings, larger numbers mean thicker lines

3.4.2.3.1 General line thickness settings

`linethickness` (setting in `colour.style`: `3`)

This determines the thickness of all lines in all plots, except for those given special values below.

3.4.2.3.2 Line thickness settings for control parameter – wave speed plots

`homocliniclinethickness` (setting in `colour.style`: 5)
: This determines the thickness of the loci of homoclinic solutions (which are actually contours of waves of large period that have been designated as homoclinic).

`hopflocuslinethickness` (setting in `colour.style`: 5)
: This determines the thickness of the loci of Hopf bifurcations in the travelling wave equations.

`periodcontourlinethickness` (setting in `colour.style`: 3)
: This determines the thickness of contours of constant period.

`sbdyeckhauslinethickness` (setting in `colour.style`: 5)
: This determines the thickness of curve(s) indicating the boundary between stable and unstable waves, when the change of stability is of Eckhaus type.

`sbdyhopflinethickness` (setting in `colour.style`: 5)
: This determines the thickness of curve(s) indicating the boundary between stable and unstable waves, when the change of stability is of Hopf type.

3.4.2.3.3 Line thickness settings for bifurcation diagram plots

`bdlinethicknessmax` (setting in `colour.style`: 3)
`bdlinethicknessmean` (setting in `colour.style`: 3)
`bdlinethicknessmin` (setting in `colour.style`: 3)
`bdlinethicknessnorm` (setting in `colour.style`: 3)
`bdlinethicknessperiod` (setting in `colour.style`: 3)
`bdlinethicknessstst` (setting in `colour.style`: 3)
: These settings determine the thickness of the curves showing the various properties of the periodic travelling wave solution branch.

3.4.2.3.4 Line thickness settings for the `@line`, `@point` and `@text` commands

`extralinethickness` (setting in `colour.style`: 1.5)
: This specifies the thickness of lines generated by the `@line` command. Note that this does not affect any other lines.

3.4.2.4 Line Type Settings

These are specified by a code number, whose interpretation depends on whether the plotter being used is `sm` or `gnuplot`. For `gnuplot`, the number specifies the `gnuplot` line style of that number. This is terminal dependent: see `gnuplot` documentation for details. In particular the same number may give different line styles on the screen and in a postscript plot. This is clearly unsatisfactory but is an intrinsic feature of `gnuplot`. However two different line style are guaranteed to be the same for all terminal types including postscript files: -1 = solid and 0 = dotted. In fact these are the only line styles available for the wxt terminal, which is the screen terminal set at installation. Therefore it is recommended

that if `gnuplot` is being used as the plotter then only solid and dotted lines are used, with different line types further distinguished by colour or by different greyscale shades. Note that the `gnuplot` line style with a particular number also carries with it a colour, but this is ignored by WAVETRAIN, being overwritten by the appropriate colour setting (specified above). For `sm`: -1 = solid, 0 = dotted, 1 = short dashed, 2 = long dash, 3 = dot & short dash, 4 = dot & long dash, 5 = short dash & long dash. Curves/lines for which no setting is listed below are always solid.

3.4.2.4.1 Line type settings for control parameter – wave speed plots

`homocliniclinetype` (setting in `colour.style`: `-1`)
: This determines the line type of the loci of homoclinic solutions (which are actually contours of waves of large period that have been designated as homoclinic).

`hopflocuslinetype` (setting in `colour.style`: `-1`)
: This determines the line type of the loci of Hopf bifurcations in the travelling wave equations.

`periodcontourlinetype` (setting in `colour.style`: `-1`)
: This determines the line type of contours of constant period.

`sbdyeckhauslinetype` (setting in `colour.style`: `-1`)
: This determines the line type of curve(s) indicating the boundary between stable and unstable waves, when the change of stability is of Eckhaus type.

`sbdyhopflinetype` (setting in `colour.style`: `-1`)
: This determines the line type of curve(s) indicating the boundary between stable and unstable waves, when the change of stability is of Hopf type.

3.4.2.4.2 Line type settings for bifurcation diagram plots

`bdlinetypemax` (setting in `colour.style`: `-1`)
`bdlinetypemean` (setting in `colour.style`: `-1`)
`bdlinetypemin` (setting in `colour.style`: `-1`)
`bdlinetypenorm` (setting in `colour.style`: `-1`)
`bdlinetypeperiod` (setting in `colour.style`: `-1`)
`bdlinetypestst` (setting in `colour.style`: `-1`)
: These settings determine the line types of curves showing the various properties of the periodic travelling wave solution branch.

3.4.2.4.3 Line type settings for the `@line`, `@point` and `@text` commands

`extralinetype` (setting in `colour.style`: `0`)
: This specifies the line type of lines generated by the `@line` command. Note that this does not affect any other lines.

Part 4

Reference Guide to WAVETRAIN

4.1 Alphabetical List of Run Commands

`add_points_list <subdirectory> <pcode>`

This command calculates the periodic travelling wave solutions and, if appropriate, their stability, for additional points in the control parameter–wave speed plane, following a previous run of `ptw_loop` or `stability_loop`. Stability will be calculated if the original run was of `stability_loop`, but not if the original run was of `ptw_loop`. The additional points are a list of control parameter and wave speed values, specified in the file `parameter_list.input` in the specified subdirectory of `input_files`. All other input files are copied from the record of those used in the original run of `ptw_loop` or `stability_loop`: the current files in the `input_files` subdirectory are not used, except for `parameter_list.input`, which must contain a list of the new points in the parameter plane. The required format is pairs of control parameter and wave speed values, separated by one or more spaces, with each pair on a separate line. Note that this command cannot be used for a pcode value generated using the `new_pcode` command. Note also that the axes limits in control parameter–wave speed plots are based on the entries in the file `parameter_range.input` at the time of the initial run of `ptw_loop` or `stability_loop`, and are unaffected by runs of `add_points_list`.

`add_points_loop <subdirectory> <pcode>`

This command calculates the periodic travelling wave solutions and, if appropriate, their stability, for additional points in the control parameter–wave speed plane, following a previous run of `ptw_loop` or `stability_loop`. Stability will be calculated if the original run was of `stability_loop`, but not if the original run was of `ptw_loop`. The additional points are a grid of control parameter and wave speed values, as specified in the file `parameter_range.input` in the specified subdirectory of `input_files`. All other input files are copied from the record of those used in the original run of `ptw_loop` or `stability_loop`: the current files in the `input_files` directory are not used, except for `parameter_range.input`. Note that this command cannot be used for a pcode value generated using the `new_pcode` command. Note also that the axes limits in control parameter–wave speed plots are based on the entries in the file `parameter_range.input` at the time of the initial run of

ptw_loop or stability_loop, and are unaffected by runs of add_points_loop.

auto97test

This command runs a test of the AUTO97 package, which is used extensively by WAVETRAIN. Typically, the command results in various compilation warnings. These warnings are compiler-dependent but typically do not cause any problems. However it is possible that the auto code will fail to compile even if the fortrantest command ran successfully, since AUTO97 departs somewhat from the Fortran77 standard. WAVETRAIN requires the user to have a Fortran77 compiler that can compile AUTO97. If compilation is successful, a test run will be performed, which will generate some numerical screen output. This should be compared with the reference output given in the user guide, which is reproduced in the file example_output in the subdirectory auto_test of the main WAVETRAIN directory.

bifurcation_diagram <subdirectory> <pname>=<pvalue>
bifurcation_diagram <subdirectory> <speedname>=<speedvalue>
bifurcation_diagram <subdirectory> variable=<name> <pname>=<pvalue>
bifurcation_diagram <subdirectory> variable=<name>
<speedname>=<speedvalue>

This command calculates the bifurcation diagram of the periodic travelling wave solutions as either the physical parameter or the wave speed are varied, with the other fixed at the value specified in the command line. The range of control parameter or wave speed values considered is that given in the file parameter_range.input. Note that the first stage of the calculation is to look for a Hopf bifurcation in the periodic travelling wave equations within this parameter range. If no Hopf bifurcation is found then the calculation terminates – this does not imply that there are no periodic travelling waves in this range, but rather that if there are waves then the Hopf bifurcation from which they arise is outside the range. Note in particular that the Hopf bifurcation limits given in equations.input are not used by this command. If a variable name is given (one of the travelling wave variable names listed in variables.input), then the properties of that variable (maximum, minimum, L2-norm, average and steady state) are written to the output files, for use in plotting. Otherwise, plotting can only be done using the L2-norm of the whole periodic travelling wave solution and/or the whole steady state solution, or the wave period. If the bifurcation_diagram command has three arguments, the second and third arguments can be given in either order.

cleanup

This command deletes various temporary files created during calculations. It is run automatically as the final stage of commands if the constant iclean (defined in constants.input) is set to 1, but it can be run manually. Specifically, the command deletes all files in the directories */cleaned_up_files, */data_files and temp_files. None of these files are needed for plotting, but it is sometimes helpful to retain them after a run for debugging purposes.

convergence_table <subdirectory> <ecode> <evalue_list>

This command displays the results of a previous run of the eigenvalue_convergence

command. The third and subsequent arguments are a list of eigenvalue numbers, between 1 and the total number of calculated eigenvalues. Alternatively `all` (or `All` or `ALL`) can be entered in place of <`evalue_list`> to give results for all of the calculated eigenvalues. The command produces a convergence table for the real and imaginary parts of the specified eigenvalues, and also lists estimated error bounds for each of these eigenvalues. Note that the error bounds are only approximate, and when one or more of the original partial differential equations do not contain time derivatives (i.e. (1.1b,c) applies) then the error bounds are particularly crude: see §3.1.10 for details. Eigenvalue numbers that are out of range (i.e. that exceed the total number of calculated eigenvalues) generate a warning but are otherwise ignored.

`copy_hopf_loci` <`subdirectory`> <`pcode1`> <`pcode2`>
: This command copies the data files corresponding to Hopf bifurcation loci from `pcode1` to `pcode2`. All loci are copied, but the hcode values may be changed so that any existing loci data files for `pcode2` are not overwritten.

`copy_period_contours` <`subdirectory`> <`pcode1`> <`pcode2`>
: This command copies the data files corresponding to contours of constant period from `pcode1` to `pcode2`. All contours are copied, but the ccode values may be changed so that any existing contour data files for `pcode2` are not overwritten.

`copy_stability_boundaries` <`subdirectory`> <`pcode1`> <`pcode2`>
: This command copies the data files corresponding to stability boundaries from `pcode1` to `pcode2`. All stability boundaries are copied, but the scode values may be changed so that any existing stability boundary data files for `pcode2` are not overwritten.

`eigenvalue_convergence` <`subdirectory`> <`pvalue`> <`speed`> <`nmesh2_list`>
: This command calculates a convergence table for eigenvalues corresponding to periodic eigenfunctions, as the computational constant `nmesh2` is varied; larger `nmesh2` values correspond to finer numerical discretisations. The intended use of this command is to determine a suitable value of `nmesh2` (set in the file `constants.input`) when calculating periodic travelling wave stability. The results of this command are displayed using the command `convergence_table`.

`fortrantest`
: This command runs a test of the Fortran77 compiler, which is a system requirement. If the resulting screen output is "`Test completed`" then the compiler has passed the test. If an error message appears, such as "`f77: Command not found`", this indicates that a compiler needs to be installed. A third possibility is that "`Test completed`" appears, but is preceded by a list of subroutines. This indicates that by default, the compiler operates in a non-silent mode. This type of compiler output will make the screen output produced by WAVETRAIN very difficult to follow, and it should be suppressed. This can be done by editting the file `input_files/defaults.input` and adding a suitable compiler flag on the line indi-

cated. The appropriate flag is compiler dependent, but "`-silent`" or "`-fsilent`" are likely possibilities.

`hopf_locus <subdirectory> <pcode> <pvalue1> <speed1> <pvalue2> <speed2>`

This command calculates a locus of Hopf bifurcation points in the travelling wave equations. The starting point for the locus is determined by searching for a Hopf bifurcation between the two specified points in the control parameter–wave speed plane. Only horizontal or vertical searches in this parameter plane are allowed, so that the arguments must satisfy either `pvalue1=pvalue2` or `speed1=speed2`.

`list_crossings <subdirectory> <pcode> <scode>`

The command `stability_boundary` allows optional arguments specifying control parameter or wave speed values for which any crossing points of the stability boundary curve are to be recorded. This command lists these crossing points. If it reports that there are no crossing points, this may either be because no optional arguments were given to the `stability_boundary` command, or because the boundary curve did not pass through the specified values.

`list_periods <subdirectory> <pcode>`

This command lists the period associated with each period contour that has been calculated.

`list_rcodes <subdirectory> <optional pcode>`

This command lists the control parameter and wave speed associated with each rcode value, plus the overall outcome of the calculation, and the period of the wave if one was found. If the value of pcode is omitted, it is taken to be 100, which corresponds to individual runs, rather than those performed via a loop through control parameter–wave speed values.

`new_pcode <subdirectory>`

This command creates a new output directory and copies the input files into this new directory. It does no calculations. The command is intended to enable Hopf bifurcation loci, period contours, and stability boundaries to be calculated without running `ptw_loop` or `stability_loop`.

`pathtest`

This command examines the search path to check whether it includes the current directory. If not, it attempts to determine which unix shell is being used, and on the basis of this produces screen output advising the user on how to change the search path. Note that because the search path might not include the current directory when this command is run, it should be entered as `./pathtest`.

`period_contour <subdirectory> <pcode> <pvalue> <speed>`
`period_contour <subdirectory> <pcode> period=<period> <pvalue1> <speed1> <pvalue2> <speed2>`

This command calculates a contour of fixed period for periodic travelling wave solutions. In the first usage, the wave is located for the given values `<pvalue>` and

<speed>, and the contour is drawn for the period of this wave. In the second usage, the contour is drawn for the specified value of the period. In this case, the periodic travelling wave with <pvalue1> and <speed1> is found, and then the starting point for the contour is determined by searching the control parameter–wave speed plane between (<pvalue1>,<speed1>) and (<pvalue2>,<speed2>), looking for a wave with the required period. Only horizontal or vertical searches in this parameter plane are allowed, so that the arguments must satisfy either pvalue1=pvalue2 or speed1=speed2. Note that it is necessary that a periodic travelling wave exists for (<pvalue>,<speed>) in the first usage, and for (<pvalue1>,<speed1>) in the second usage. However, it is not necessary for there to be a wave for (<pvalue2>,<speed2>) in the second usage. In both usages, the computational constant iwave is used (see §3.1.8 for details), and it is required that the periodic travelling wave branch does not have a fold between (<pvalue1>,<speed1>) and (<pvalue2>,<speed2>): no check is made on this during execution.

plot <subdirectory> <optional pcode>
: This command runs the plotter. If the value of pcode is omitted, it is taken to be 100, which corresponds to individual runs, rather than those performed via a loop through the control parameter–wave speed plane.

ptw <subdirectory> <pvalue> <speed>
: This command calculates the periodic travelling wave solution for the specified values of the control parameter and wave speed. Stability of the wave is not calculated.

ptw_loop <subdirectory>
: This command calculates the periodic travelling wave solutions for a grid of points in the control parameter–wave speed plane, as specified in parameter_range.input. Stability of the waves is not calculated.

rmbcode <subdirectory> <bcode>
rmbcode <subdirectory> all
: This command deletes all output files associated with the bifurcation diagram calculation with the specified bcode value, and also deletes the corresponding output directory. If the second argument is all (All and ALL are also allowed), then the files and directories associated with all bcode values are deleted.

rmccode <subdirectory> <pcode> <ccode>
rmccode <subdirectory> <pcode> all
: This command deletes all output files associated with the period contour calculation with the specified ccode value, and also deletes the corresponding output directory. If the second argument is all (all and ALL are also allowed), then the files and directories associated with all ccode values are deleted.

rmecode <subdirectory> <ecode>
rmecode <subdirectory> all
: This command deletes all output files associated with the eigenvalue convergence calculation with the specified ecode value, and also deletes the corresponding output

directory. If the second argument is `all` (`all` and `ALL` are also allowed), then the files and directories associated with all ecode values are deleted.

`rmhcode <subdirectory> <pcode> <hcode>`
`rmhcode <subdirectory> <pcode> all`
This command deletes all output files associated with the Hopf bifurcation locus calculation with the specified hcode value, and also deletes the corresponding output directory. If the second argument is `all` (`all` and `ALL` are also allowed), then the files and directories associated with all hcode values are deleted.

`rmpcode <subdirectory> <pcode>`
`rmpcode <subdirectory> all`
This command deletes all output files associated with all calculations for the specified pcode value, and also deletes the corresponding output directory. If the second argument is `all` (`all` and `ALL` are also allowed), then the files and subdirectories associated with all pcode values are deleted, followed by the (empty) output directory for `<subdirectory>`. Various prompts are issued to confirm that the user wishes to proceed.

`rmrcode <subdirectory> <rcode>`
`rmrcode <subdirectory> <pcode> <rcode>`
This command deletes all output files associated with the periodic travelling wave calculation with the specified rcode value, and also deletes the corresponding output directory. If no pcode value is specified then pcode is set to 100, corresponding to calculations that are run individually, rather than as part of a parameter plane loop. If pcode is greater than 100, the list of convergence failures is also updated.

`rmscode <subdirectory> <pcode> <scode>`
`rmscode <subdirectory> <pcode> all`
This command deletes all output files associated with the stability boundary calculation with the specified scode value, and also deletes the corresponding output directory. If the second argument is `all` (`all` and `ALL` are also allowed), then the files and directories associated with all scode values are deleted.

`set_homoclinic <subdirectory> <pcode> <ccode>`
This command designates the period contour with the specified ccode value as being a homoclinic solution. There is no facility within WAVETRAIN to calculate the true loci of homoclinic solutions: rather these must be approximated by the loci of solutions with constant (large) period. This command should be used after a locus of large period has been calculated. It does not involve any new computation: it is just a change of labelling that effects the way in which the contour is plotted. Its effect can be reversed by the command `unset_homoclinic`. If the contour has already been designated as homoclinic then no error is reported, but the command has no effect.

`set_worked_example_inputs <stage>`
This command performs the various input stages of the worked example described

in §2.3, up to and including the specified stage. Thus for example the command "set_worked_example_inputs 5" first empties the workedex input subdirectory (if it exists) and then performs the various steps in stages 1, 3 and then 5 of the worked example.

stability <subdirectory> <pvalue> <speed>

This command calculates the periodic travelling wave solution for the specified values of the control parameter and wave speed, and then calculates its stability.

stability_boundary <subdirectory> <pcode> <pvalue1> <speed1>
<pvalue2> <speed2> <optional arguments>

This command calculates a curve separating regions of stable and unstable periodic travelling waves. The starting point for the curve is determined by searching for a change in stability between the two specified points in the control parameter–wave speed plane. Only horizontal or vertical searches in this parameter plane are allowed, so that the arguments must satisfy either pvalue1=pvalue2 or speed1=speed2. The optional arguments have the form <control_parameter_name>=<value> or <wave_speed_name>=<value>; if present, the program records any points at which the stability boundary crosses the specified values. These crossing points can be listed using the list_crossings command; they are not used in plotting. Note that the computational constant iwave applies to calculations done using this command (see §3.1.8 for details), and it is required that the periodic travelling wave branch does not have a fold between (<pvalue1>,<speed1>) and (<pvalue2>,<speed2>): no check is made for this during execution. *Warning:* this calculation can be quite time-consuming. It may be helpful to experiment with the stability command in order to obtain starting points in the control parameter–wave speed plane that are relatively close together (and are on either side of the stability boundary). The trade-off in computation time between such experiments and a longer run of stability_boundary is dependent on the problem and on the various input parameters set in the file constants.input.

stability_loop <subdirectory>

This command calculates the periodic travelling wave solutions, and their stability, for a grid of points in the control parameter–wave speed plane, as specified in the file parameter_range.input.

unset_homoclinic <subdirectory> <pcode> <ccode>

This command designates the period contour with the specified ccode value as not being a homoclinic solution, reversing the effect of a previous use of the command set_homoclinic. If the contour has not previously been designated as homoclinic then no error is reported, but the command has no effect.

wt_help <command>

This command gives a brief description of the syntax and use of the specified command, which can be either a run command or a plot command. If no argument is given, then the available run and plot commands are listed.

4.2 Alphabetical List of Plot Commands

`@bd <bcode>`
: This is an abbreviation for `@bifurcation_diagram`.

`@bifurcation_diagram <bcode>`
: These commands plot the bifurcation diagram associated with the specified bcode value. The user will be prompted to enter what should be plotted on the vertical axis (wave period, L2-norm of the solution etc.). The limits on the vertical axis are chosen based on the whole data file, but the user will be given an opportunity to override these limits; this is particularly useful when plotting the period close to parameter values for which there is a homoclinic solution. When the user selects to plot only one solution measure, the plot will only contain a single curve, making a key unnecessary, but in other cases the plot includes a key, showing the meaning of the various line types.

`@exit`
: This command deletes some temporary files before exitting from the plotter. It is equivalent to the command `@quit`.

`@help <optional command>`
: This command provides a brief summary of the syntax and use of the specified command. If no argument is given then a list of plot commands is displayed.

`@hl <hcode>`
`@hl all`
: This is an abbreviation for `@hopf_locus`.

`@hopf_locus <hcode>`
`@hopf_locus all`
: These commands plot the Hopf bifurcation locus associated with the specified hcode value, or with all hcode values if the argument is `all` (`All` and `ALL` are also allowed).

`@line <x_coordinate1> <y_coordinate1> <x_coordinate2> <y_coordinate2>`
: This command draws a line between the two specified points. When plotting with `gnuplot` (but not `sm`), negative coordinates must be enclosed in double quotes, e.g. `"-1.2"`.

`@linesfile <file_name>`
: This command plots a series of line segments connecting the points given in the first two columns of the specified file, which must be located in the relevant input subdirectory. The data file can contain more than two columns: other columns will be ignored.

`@pc <ccode>`
`@pc all`
: This is an abbreviation for `@period_contour`.

`@period_contour <ccode>`

`@period_contour all`

These commands plot the period contour associated with the specified <`ccode`> value, or with all ccode values if the argument is `all` (`All` and `ALL` are also allowed).

`@point <x_coordinate> <y_coordinate>`

This command draws a single dot (or other symbol, as defined by `extrapointtype` in the plotter style file) at the specified location.

`@pointsfile <file_name> <point_type>`

This command plots a series of dots (or other symbols) at the location specified by the first two columns of the specified file, which must be located in the relevant input subdirectory. The second argument specifies the symbol type. The meanings of the symbol type code numbers are given on page 127 and also in the comments of the style file(s). The data file can contain more than two columns: other columns will be ignored.

`@postscript <filename>`

These commands cause subsequent plotter commands to be written to the file <`filename`>`.eps` in the appropriate subdirectory of `@postscript_files`. If the plotter setting `keeprecords` is set to `yes`, the command also causes the plotter command record file <`filename`>`_record/`<`filename`>`.plt` and the run command and data record archive <`filename`>`_record/`<`filename`>`.tar` to be generated, which contain full details of the plotter commands and output data (respectively) that were used to create the plot. Note that plot commands are actually written to a buffer, and are only output to the postscript file when either the plotter device is changed (usually with either the `@screen` command, or with another `@ps` or `@postscript` command), or when the plotter is exitted (via the `@exit` or `@quit` command).

`@pp`

This is an abbreviation for `@pplane`.

`@pplane`

This command plots the control parameter–wave speed plane, indicating the existence of periodic travelling waves, and their stability if that has been calculated. There are three different plot types, denoting the waves by their rcode numbers, their periods, or a symbol. The default is set in `plot_defaults.input`, and the user is asked whether to use this default or override it. A key to the colours and symbols used in this plot is given in the file `postscript_files/pplane_key.eps`; the key also shows the colours and styles of curves that may be added by subsequent plot commands. This file is regenerated each time the plotter is started, and also whenever the `@set_style` command is used; the choice of which symbols/lines are included in the key is specified in `plot_defaults.input`.

`@ps <filename>`

This is an abbreviation for `@postscript`.

`@ptw <rcode>`
: This command plots the periodic travelling wave solution, as a function of the travelling wave coordinate, for the specified value of rcode.

`@quit`
: This command deletes some temporary files before exitting from the plotter. It is equivalent to the command `@exit`.

`@sb <scode>`
`@sb all`
: This is an abbreviation for `@stability_boundary`.

`@screen`
: This command sets the plotter to write to the screen, and clears the plotting area (i.e. it starts a new plot). This is typically used to begin a new screen plot after plotting to a postscript file. If the plotter being used is `gnuplot`, "the screen" denotes whatever is set as the plotting terminal in `plot_defaultsinput`. If the plotter being used is `sm`, "the screen" denotes whatever is set as the default plotter device in the user's `.sm` file.

`@set_style <style_name>`
: This command sets the default colours, line thicknesses and line styles, by reading them from `<style_name>.style` (in the `input_files` directory). It then regenerates the postscript file containing the key to the lines and symbols used in plots of the control parameter–wave speed plane. For this reason, if a postscript file is currently being written then it is ended by the `@set_style` command, with plotting returned to the screen at the end of the command.

`@sp <rcode>`
: This is an abbreviation for `@spectrum`.

`@spectrum <rcode>`
: This command plots the eigenvalue spectrum for the periodic travelling wave solution corresponding to the specified value of rcode; if stability was not calculated for that value of rcode, then an error is reported. If `spectrumcolour` (defined in the plotter style file) is set to "`rainbow`" or "`greyscale`" (or "`grayscale`") then a key for interpreting the colours is included in the plot.

`@stability_boundary <scode>`
`@stability_boundary all`
: This command plots the stability boundary associated with the specified scode value, or with all scode values if the argument is `all` (`All` and `ALL` are also allowed). The boundary can correspond to a change in stability of either Eckhaus or Hopf type, and this is indicated by the colour and/or style of the line.

`@text <x_coordinate> <y_coordinate> <text_string>`
: This command writes a piece of text (which must be in double quotes if it contains spaces) centred at the specified point.

4.3 WAVETRAIN Directory Structure

4.3.1 The Structure of Subdirectories of the Main WAVETRAIN Directory

For the benefit of users wanting to delve into the inner workings of WAVETRAIN, this section summarises the overall directory structure of the WAVETRAIN code. The main WAVETRAIN directory contains a formal copyright and disclaimer statement in the file `COPYRIGHT_DISTRIBUTION_DISCLAIMER`, plus a file `README` containing the WAVETRAIN version name/ number. All other files in this directory are relatively simple Bourne shell scripts for the various commands. Most of the WAVETRAIN code is divided into a series of subdirectories:

`auto_code` This subdirectory contains the required parts of AUTO97. Some very minor changes have been made to the AUTO code, mainly removal of the "unknown" file status, for consistency with other Fortran77 programs in WAVETRAIN. The command names have also been altered, so that for example the standard AUTO command `@r` has been replaced by `auto_r`. This prevents any interference with existing AUTO code for users who have previously installed AUTO. At the start of each run command, a check is made on the AUTO files `auto_code/include/auto.h` and `auto_code/include/fcon.h` to see whether the AUTO code needs to be recompiled: each run of WAVETRAIN is performed using the smallest possible values of the AUTO constants NINTX, NDIMX, NBCX and NTSTX, in order to reduce run times.

`auto_test` This subdirectory contains files associated with the command `auto97test`.

`cleaning_up` This subdirectory contains the shell scripts associated with the deletion of data files (see §3.1.6).

`controller` This subdirectory contains the basic shell scripts and a few associated files for all of the WAVETRAIN commands. These scripts control the overall structure of the commands; for example the `period_contour` command is controlled primarily by the file `periodcontour.script` which runs various programs contained in the `loci` subdirectory.

`documentation` This subdirectory contains a PDF file of this user guide. It also contains a sub-subdirectory `worked_example` containing files associated with the command `set_worked_example_inputs`.

`gammazero` This subdirectory contains files associated with the calculation of eigenvalues corresponding to periodic eigenfunctions.

`help_files` This subdirectory contains files associated with the help system for run commands. Note the plotter help files are stored separately, in `plotting/help_files`.

`input_files` This subdirectory was discussed extensively in §2.2. It contains the two files `defaults.input` and `plot_defaults.input`, plotter "style" files which have the extension `.style`, and a series of sub-subdirectories, each of which contains input files associated with a particular set of equations.

`loci` This subdirectory contains files associated with the calculation of the Hopf bifurcation loci, contours of constant wave period, and stability boundaries.

`managing_info` This subdirectory contains all files associated with the writing of information and error messages to output files and the screen.

`output_files` This subdirectory will be discussed in detail in §4.4. It contains a series of sub-subdirectories, each of which contains output files associated with a particular set of equations. It also contains two files. The file `logfile` contains the code numbers of any runs performed with `info`=1. This setting is intended for background runs, and no output is written to the screen; the code numbers are needed in order to plot the results. Each successive entry to `logfile` is simply appended to the current file (or the file is created if it does not exist), and the file can be emptied or deleted by the user whenever convenient. The second file in the `output_files` subdirectory is `README`, which gives the version of WAVETRAIN being used (e.g. `wavetrain1.0`).

`plotting` This subdirectory contains all programs associated with the WAVETRAIN plotter. General plotting programs are located in this subdirectory itself, while macros associated with a particular plotter (gnuplot or sm) are in sub-subdirectories. The sub-subdirectory `help_files` contains the files associated with the plotter's help system. There is also a sub-subdirectory `temp_files`, which contains temporary data files generated during plotting; these are deleted by the `@quit` or `@exit` commands.

`postscript_files` This subdirectory contains the single file `colour_list.eps` (see §3.3.1), plus a series of subdirectories containing postscript files associated with runs of the `plot` command.

`processing` This subdirectory contains the shell scripts and text files that are used to process the files `variables.input` and `equations.input`. The scripts convert the file `variables.input` into a more usable form, and convert the file `equations.input` into Fortran77 code. There is also a sub-subdirectory `most_recent_run`, which contains details of the `equations.input` file and associated constants that were last converted to Fortran77. This is checked whenever a new run command is entered, to determine whether processing must be redone.

`ptwcalc` This subdirectory contains files associated with the calculation of periodic travelling wave existence and form, and also those associated with `bifurcation_diagram` calculations.

`spectrum` This subdirectory contains files associated with the calculation of the portions of the spectrum in between the eigenvalues corresponding to periodic eigenfunctions.

`temp_files` This subdirectory is a "dumping ground" for temporary files created during runs. The directory is emptied at the end of runs if `iclean` (set in `constants.input`) has the value 1. The files are not needed for plotting, but users wishing to retain them for debugging can do so by setting `iclean`=2.

The subdirectories `controller`, `gammazero`, `loci`, `ptwcalc` and `spectrum` all contain sub-subdirectories named `cleaned_up_files` and `data_files`, which are used as repositories for temporary files generated during runs. Roughly, the <`subdir`>`/cleaned_up_files` sub-subdirectories contain temporary program files, while the <`subdir`>`/data_files` sub-subdirectories contain temporary data files used mainly by programs in <`subdir`>, and `temp_files` contains temporary data files used in a variety of different subdirectories. Like `temp_files`, the `cleaned_up_files` and `data_files` sub-subdirectories are emptied at the end of each run if `iclean` (set in `constants.input`) has the value 1. The files are not needed for plotting, but users wishing to retain them for debugging can do so by setting `iclean`=2 in `constants.input`.

4.4 Details of Output Data Files

In normal use, there is no need for the user to be concerned with the data files generated by WAVETRAIN: in particular, this is not required in order to visualise the results using the plotter. However, occasionally users may wish to export data from WAVETRAIN calculations into other software. To assist in this, this section summarises the structure of the WAVETRAIN `output_files` directory, and gives details of the data files that will be present in the various output subdirectories after runs of WAVETRAIN commands. The information on output files applies to cases in which runs have been successful and periodic travelling waves have been detected: for instance, if a run of `ptw` does not find a periodic travelling wave, then clearly the data files associated with periodic travelling wave form will not be present.

4.4.1 The Directory Structure of WAVETRAIN Output

Output data falls into two basic categories: (i) data that is associated with control parameter–wave speed planes; (ii) data this is not associated with control parameter–wave speed planes. Output in category (i) is all associated with a particular pcode value (101–999), and it is stored in the directory `output_files/pcode`<`code_number`>. Within such a directory, there are a small number of data files, which are copies of the input files as they were when the directory was created. The remainder of the data is stored in a series of subdirectories:

`output_files/pcode`<`code_number`>`/ccode`<`code_number`>
: contains data on calculations of the contour of constant wave period with the specified code number.

`output_files/pcode`<`code_number`>`/hcode`<`code_number`>
: contains data on calculations of the Hopf bifurcation locus associated with the specified code number.

`output_files/pcode`<`code_number`>`/rcode`<`code_number`>
: contains data on calculations of periodic travelling wave existence, form and possibly

stability. Note that rcode numbers are four digits (1001-9999) while all other code numbers in WAVETRAIN are three digits.

`output_files/pcode<code_number>/scode<code_number>`
: contains data on calculations of the stability boundary with the specified code number.

Details of the files in these various subdirectories are given in the following subsections.

Data in category (ii) is all stored in the directory `output_files/pcode100`. Note that 100 is not a valid pcode value for a parameter plane run (which must have a pcode between 101 and 999); the directory name `pcode100` is simply chosen for compatibility. There are no files directly in the `pcode100` directory: all files are in subdirectories, which are of three possible types:

`output_files/pcode100/bcode<code_number>`
: contains data on calculations associated with bifurcation diagrams with the specified code number.

`output_files/pcode100/ecode<code_number>`
: contains data on eigenvalue convergence calculations associated with the specified code number.

`output_files/pcode100/rcode<code_number>`
: contains data on calculations of periodic travelling wave existence, form and (possibly) stability associated with the specified (four digit) code number. These are runs done using either the command `ptw` or the command `stability`.

All of these various directories are created by WAVETRAIN as required. Thus if the first run of a WAVETRAIN command using the input directory `demo` (say) is `ptw`, then this command creates the directories `output_files/demo`, `output_files/demo/pcode100` and `output_files/demo/pcode100/rcode1001`; the next run of the same command will create just `output_files/demo/pcode100/rcode1002`.

Although all code numbers of a particular type are created sequentially, gaps can arise via the file deletion commands (see §3.1.6). For example, the first three runs of `bifurcation_diagram` for input directory `demo` will create the directories `output_file/demo/pcode100/bcode1001`, `output_file/demo/pcode100/bcode1002` and `output_file/demo/pcode100/bcode1003`. If the command

```
rmbcode demo 1002
```

is given, then the second of these three output directories will be deleted. A subsequent run of `bifurcation_diagram` will then "fill the gap" by re-creating the directory `output_file/demo/pcode100/bcode1002`.

4.4.2 pcode Subdirectories

As discussed in §4.3.1, all output data is contained in a subdirectory of a directory named `pcode<value>`, where "`value`" is in the range 100-999. The `pcode100` contains subdirectories with data files associated with runs of the commands `bifurcation_diagram`,

eigenvalue_convergence, ptw and stability; there are no files in the pcode100 directory itself. Directories pcode101–pcode999 contain data associated with studies of control parameter–wave speed parameter planes. These directories themselves contain copies of the input files, and also the following files:

equations.f This is the Fortran77 file that is generated using equations.input and that forms the basis of all WAVETRAIN calculations. It is included simply as a reference for any users wishing to see the source code used by WAVETRAIN.

errors.txt If any errors or warnings occur during the run, they will be listed in this file; otherwise the file will be present but empty. Note that this file contains a compilation of all error and warning messages that are generated during all runs associated with the pcode value. The messages are duplicated in the errors.txt file in the relevant subdirectory (see below).

info.txt This file contains information on the run of whichever of new_pcode, ptw_loop or stability_loop created the subdirectory. This file itself contains only general information about the progression through the command: detailed information is contained in the separate rcode subdirectories. If the command add_points_list or add_points_loop has been run for this pcode value, then corresponding general information will be appended to this file.

onlyptw.data This file contains the character n or the character y, indicating (respectively) whether stability was or was not determined for runs with this pcode value. This file will not be present if the pcode directory was generated using the new_pcode command.

The computational output data itself is contained in a directory of one of six types: bcode<value>, ecode<value> (which are subdirectories of output_files/<subdir>/-pcode100/), ccode<value>, hcode<value>, scode<value> (which are subdirectories of output_files/<subdir>/pcode101/,..., output_files/<subdir>/pcode999/), and rcode<value> (which can be subdirectories of any pcode output directory). These six subdirectory types all contain copies of the input files, and also all contain the following files:

command.txt This one-line file contains the WAVETRAIN command (with arguments) that generated the directory. This file is not present in rcode<value> subdirectories for pcode values 101-999, since these are not generated directly by a WAVETRAIN command; however it is present in rcode<value> subdirectories for pcode 100, and for all cases of the other five types of output subdirectory.

equations.f This is the Fortran77 file that is generated using equations.input and that forms the basis of all WAVETRAIN calculations. It is included simply as a reference for any users wishing to see the source code used by WAVETRAIN.

errors.txt If any errors or warnings occur during the run, they will be listed in this file; otherwise the file will be present but empty.

`info.txt` This file contains detailed information on the run. It is the key to understanding any unexpected results during the run; this file and `errors.txt` are the only output files that users are expected to want to access unless they are exporting data from WAVETRAIN. Note that the contents of `errors.txt` is replicated in `info.txt`.

The remainder of this section documents the other files that are present in the six types of output directory.

4.4.3 bcode Subdirectories

These are associated with calculations of bifurcation diagrams. After a successful run of the `bifurcation_diagram` command, the following files will be present:

`bd.data` This is the main data file containing the calculated points along the period contour.

Column 1: the bifurcation parameter, which can be either the control parameter or the wave speed.

Column 2: the norm of the whole wave solution.

Column 3: the wave period.

Column 4: the maximum of the selected variable.

Column 5: the mean of the selected variable.

Column 6: the minimum of the selected variable.

Column 7: the norm of the selected variable.

Column 8: 1 or 0, according to whether this line is a genuine data point or a dummy line, indicating a break in the curve. Such dummy lines are used to separate different branches of periodic travelling wave solutions, associated with different Hopf bifurcations. If this column contains 0 then the data in the other columns is irrelevant.

Columns 4–7 are only relevant if the `bifurcation_diagram` command used the optional argument "`variable=`": otherwise they contain the specified information for the first travelling wave variable listed in `variables.input`, but they are not used.

`bd.stst` This file contains the calculated value of the steady state from which periodic travelling waves bifurcate.

Column 1: the bifurcation parameter, which can be either the control parameter or the wave speed.

Column 2: the norm of the steady state.

Column 3: the steady state value of the selected variable.

Column 4: 1 or 0, according to whether this line is a genuine data point or a dummy line, indicating a break in the curve. Such dummy lines are used to delimit separate regions of steady state existence. If this column contains 0 then the data in the other columns is irrelevant.

Column 3 is only relevant if the `bifurcation_diagram` command used the optional argument "`variable=`": otherwise it contains the specified information for the first travelling wave variable listed in `variables.input`, but this is not used.

`hb_and_folds.data` This file contains information used to label Hopf bifurcation points, folds and end points on the bifurcation diagram.

Column 1: the bifurcation parameter, which can be either the control parameter or the wave speed.

Column 2: the norm of the whole wave solution.

Column 3: the wave period.

Column 4: the maximum of the selected variable.

Column 5: the mean of the selected variable.

Column 6: the minimum of the selected variable.

Column 7: the norm of the selected variable.

Columns 8 and above: a code number and explanatory text string indicating the label type: it is either "1 HOPF BIFN POINT", "2 FOLD" or "3 END OF SOLN BRANCH".

`variable.data` This file contains information about the specification of a plotting variable using the "`variable=`" option in the `bifurcation_diagram` command.

Line 1: the number of the selected variable (variables are ordered as listed in the `variables.input` file), or 1 if "`variable=`" was not used.

Line 2: the number of the selected variable (variables are ordered as listed in the `variables.input` file), or 0 if "`variable=`" was not used. This line indicates whether or not "`variable=`" was used.

Line 3: the name of the selected variable, or `L2norm` if "`variable=`" was not used.

Line 4: the name of the bifurcation parameter (which will either be the name of the control parameter or the name of the wave speed, as given in `variables.input`).

Line 5: the equality fixing whichever of the control parameter or wave speed is not the bifurcation parameter, as it appears in the command line.

4.4.4 ccode Subdirectories

These are associated with calculations of contours of constant wave period. After a successful run of the `period_contour` command, the following files will be present:

`outcome.data` This file contains a code number (the "outcome code") indicating the outcome of the calculation, followed by comments explaining the meanings of the various possible outcome codes.

`periodcontour.contourdata` This is the main data file containing the calculated points along the period contour.

Column 1: the control parameter.

Column 2: the wave speed.

Column 3: 1 or 0, according to whether this line is a genuine data point or a dummy line, indicating a break in the curve. Such a dummy line will always be present in the middle of the file, since the locus is calculated in two parts, corresponding to the two possible continuation directions at the calculated starting point. If this column contains 0 then the data in the other columns is irrelevant.

Column 4: always the two characters `hc`.

Column 5: 1 or 0, according to whether the period contour has or has not been designated as a homoclinic solution (see §3.1.3).

Column 6: the period of the wave.

`periodcontour.labels` If labelling of period contours is selected as a plot option, then by default, labels are placed where (and if) the contours intersect the edge of the plotting region. This file contains the data used to plot these labels. Note that if the user overrides the default labelling when running the plot command `period_contour`, then this file will not be used. The contents of the file are:

Column 1: the control parameter.

Column 2: the wave speed.

Column 3: an orientation code specifying where the label is to be placed relative to the point specified in columns 1 and 2.

Column 4: the period of the wave.

Column 5: always the two characters `hc`.

Column 6: 1 or 0, according to whether the period contour has or has not been designated as a homoclinic solution (see §3.1.3).

`period.data` This one-line file contains the ccode value, the period of the contour, the outcome code, and then either "`hc 0`" or "`hc 1`", indicating that the contour has not or has (respectively) been designated as homoclinic solution (see §3.1.3).

4.4.5 ecode Subdirectories

These are associated with eigenvalue convergence calculation. After a successful run of the `eigenvalue_convergence` command, the following files will be present:

`control_parameters.data` This two-line file lists the parameter values specified in the command line.

Row 1: the control parameter.

Row 2: the wave speed.

`convergence.table` This is the main data file used by the `convergence_table` command to generate convergence information.

Column 1: the value of `nmesh2`. The numbers in this column will be those given in arguments 4 and above in the command line.

Columns 2 and above: the real and imaginary parts of the eigenvalues corresponding to periodic eigenfunctions, and the estimated bound on the error in the eigenvalue. Thus the file has (1+3×`nevalues`) columns in total. Columns 2 and 3 containing the real and imaginary parts of the eigenvalue with largest real part, and column 4 contains the estimated error bound for this eigenvalue. Columns 5 and 6 containing the real and imaginary parts of the eigenvalue with the next largest real part, and column 7 contains the estimated error bound for this eigenvalue, etc. Note that output will include either all eigenvalues or just those with non-negative real part, according to the value of `iposre` (which is set in `constants.input`). Note also that the error bounds are only approximate, and when one or more of the original partial differential equations do not contain time derivatives (i.e. (1.1b,c) applies) then the error bounds are particularly crude: see §3.1.10 for details.

`number_of_eigenvalues.data` This file contains only one number: (100+`nevalues`). Note that `nevalues` is set in `constants.input`.

4.4.6 hcode Subdirectories

These are associated with calculations of Hopf bifurcation loci. After a successful run of the `hopf_locus` command, the following files will be present:

`hopflocus.locusdata` This is the main data file containing the calculated points along the Hopf bifurcation locus.

Column 1: the control parameter.

Column 2: the wave speed.

Column 3: 1 or 0, according to whether this line is a genuine data point or a dummy line, indicating a break in the curve. Such a dummy line will always be present in the middle of the file, since the locus is calculated in two parts, corresponding to the two possible continuation directions at the calculated starting point. If this column contains 0 then the data in the other columns is irrelevant.

`hopf.startdata` This one-line file contains the two pairs of control parameter and wave speed values specified in the command line.

`outcome.data` This file contains a code number (the "outcome code") indicating the outcome of the calculation, followed by comments explaining the meanings of the various possible outcome codes.

4.4.7 rcode Subdirectories

These are associated with calculations of periodic travelling waves. They are generated by one of the four commands `ptw`, `stability`, `ptw_loop`, or `stability_loop`. In the first two cases, the parent directory will be `pcode100`, and in the third and fourth cases the parent directory will be `pcode101`–`pcode999`. If the subdirectory is generated using the `ptw` or `ptw_loop` command, with a periodic travelling wave being detected, then the following files will be present:

`accurate_ptw.params` This one line file contains parameters associated with the travelling wave solution.

Column 1: the control parameter.

Column 2: the wave speed.

Column 3: the period of the travelling wave solution.

Column 4: the number of points in the travelling wave solution. (This is the number of lines in the file `accurate_ptw.soln`).

`accurate_ptw.soln` This is the main data file containing the calculated periodic travelling wave solution. The solution that is recorded is the one calculated using `nmesh1`, which can be greater than `nmesh2` (these constants are set in `constants.input`).

Column 1: the travelling wave variable divided by the period. Therefore this column ranges from 0.0 to 1.0 in all cases.

Columns 2 and above: the solution components of the periodic travelling wave, in the order that they are listed in `variables.input`.

`control_parameters.data` This file contains key parameter values.

Row 1: the control parameter value.

Row 2: the wave speed value.

Row 3: the pcode value (100-999).

Row 4: the rcode value (1001-9999).

`outcome.data` This file contains a code number (the "outcome code") indicating the outcome of the calculation, followed by comments explaining the meanings of the various possible outcome codes.

An rcode subdirectory generated using the `stability` or `stability_loop` command, with a periodic travelling wave being detected and with stability calculated successfully, contains the files listed above, and also the following additional files:

`evalues.data` This file contains the eigenvalues corresponding to periodic eigenfunctions.

Column 1: the real part of the eigenvalue.

Column 2: the imaginary part of the eigenvalue.

Column 3: a convergence code. If continuation along the spectrum starting from this eigenvalue is successful, the code is 0. Continuation along the spectrum is done in four stages: (1) continuation in a dummy parameter to obtain a suitable starting solution for the eigenfunction; (2) continuation for a few steps to establish the correct direction for continuation; (3) continuation backwards to obtain a starting point for which the phase shift in the eigenfunction is zero; (4) continuation to calculate the spectrum. If there is a convergence error during any of these stages, then the calculation terminates and the stage number in which the error occurred is written to this column. WAVETRAIN will then move on and begin continuation starting from the next eigenvalue corresponding to a periodic eigenfunction. Note that convergence errors typically occur because the discretisation used to calculate the eigenvalues corresponding to periodic eigenfunctions is too coarse, so that these eigenvalues are poor approximations to the true eigenvalues. Usually the remedy is to increase `nmesh2`, `nmesh3` or `order`.

Column 4: a code number for the eigenvalue, which ranges from 101 up to (100+ `nevalues`).

Column 5: the estimated error bound for the eigenvalue. Note that the error bound is only approximate, and when one or more of the original partial differential equations do not contain time derivatives (i.e. (1.1b,c) applies) then the error bound is particularly crude: see §3.1.10 for details.

The eigenvalues are ordered in decreasing size of their real part.

`failures.list` This file contains a list of the eigenvalues corresponding to periodic eigenfunctions for which there was a convergence error in the spectrum continuation starting from that eigenvalue.

Column 1: the control parameter.

Column 2: the wave speed.

Column 3: the real part of the eigenvalue that was the starting point for continuation.

Column 4: the imaginary part of the eigenvalue that was the starting point for continuation.

Column 5: the continuation stage during which the convergence error occurred (=1, 2, 3 or 4) (see description of column 4 of `evalues.data`).

`spectrum.max` This one-line file contains data on the fold in the eigenvalue spectrum with largest real part, away from the origin.

Column 1: the real part of the eigenvalue at the fold.

Column 2: the imaginary part of the eigenvalue at the fold.

Column 3: the phase difference in the eigenfunction across one period of the wave, at the fold.

Column 4: the real part of the eigenvalue that was the starting point for continuation of the portion of the spectrum containing the fold. (This eigenvalue corresponds to a periodic eigenfunction).

Column 5: the imaginary part of the eigenvalue that was the starting point for continuation of the portion of the spectrum containing the fold. (This eigenvalue corresponds to a periodic eigenfunction).

Column 6: the code number of the eigenvalue that was the starting point for continuation of the portion of the spectrum containing the fold. The code numbers range from 101 up to (100+`nevalues`) (see description of column 4 of `evalues.data`).

If no folds are detected away from the origin in the calculated part of the spectrum, all columns contain zero.

`spectrum.plotdata` This is the main data file containing the calculated spectrum.

Column 1: the real part of the eigenvalue.

Column 2: the imaginary part of the eigenvalue.

Column 3: 1 or 0, according to whether this line is a genuine data point or a dummy line, indicating a break in the curve. If this column contains 0 then the data in the other columns is irrelevant.

Column 4: the phase difference in the eigenfunction across one period of the periodic travelling wave.

4.4.8 scode Subdirectories

These are associated with calculations of stability boundaries. After a successful run of the `stability_boundary` command, the following files will be present:

`crossings.data` Each line of this file is a sentence documenting a point at which the stability boundary curve crosses one of the control parameter or wave speed values specified via the optional arguments in the command line (see §3.1.2). If no optional arguments were given, or if optional arguments were given but no crossings were detected, then the file will be present but empty.

`outcome.data` This file contains either one or two code numbers (the "outcome code(s)") indicating the outcome of the calculation, followed by comments explaining the meanings of the various possible outcome codes. If there is one code number, this refers to change of stability of Eckhaus type, and the number refers to the detection and tracing of the Eckhaus stability boundary curve. If there are two code numbers, this indicates that the search for a change of stability of Eckhaus type was completed

without error but without finding an Eckhaus point, so that WAVETRAIN moved on to look for a change in stability of Hopf type. This is done first starting from the control parameter and wave speed values given in the third and fourth arguments, and then (if that is unsuccessful) starting from the control parameter and wave speed values given in the fifth and sixth arguments. The two code numbers refer to the outcomes of these two calculations; the second code number is zero if the second calculation is not done, which will occur if the first calculation successfully detects and calculates a stability boundary curve.

`stabilityboundary.boundarydata` This is the main data file containing the calculated points along the stability boundary.

Column 1: the control parameter.

Column 2: the wave speed.

Column 3: 0, 1 or 2. The value 0 denotes a dummy line, indicating a break in the curve; in this case the data in the other columns is irrelevant. Such a dummy line will always be present in the middle of the file, since the locus is calculated in two parts, corresponding to the two possible continuation directions at the calculated starting point. The value 1 or 2 indicates that this is a genuine data point, with the change in stability being of Eckhaus or Hopf type respectively.

Appendix: Commands Used to Generate Figures

This Appendix lists the various run and plot commands used to generate the graphical figures in this user guide. The code numbers assume that no previous runs have been performed, and that the commands are run in order. Therefore, for each command, it is assumed that all previous run commands listed in the table have been run. It is also assumed that after plotting each figure, the plotter is exitted by typing either `@exit` or `@quit`. In all of these plots the default setting of `rainbow` is used for `spectrumcolour`. Consequently, if the plots are done using `gnuplot` rather than `sm`, there is an additional plotting option in which the user can alter the overall scaling of the plot. In all cases, the default scaling is appropriate.

Figure	Run commands	Plot commands	Plot options
2.2a	`ptw demo 2.0 1.0` `plot demo`	`@ptw 1001`	
2.2b	`ptw demo 1.5 0.8` `plot demo`	`@ptw 1002`	
2.3a	`ptw_loop demo` `plot demo 101`	`@pplane`	Plot type: `rcode`
2.3b	`plot demo 101`	`@pplane`	Plot type: `period`

2.5	`hopf_locus demo 101 2.0 0.8 3.5 0.8`
	`period_contour demo 101 period=3000 1.5 0.8 0.0 0.8`
	`period_contour demo 101 period=80 2.5 0.8 0.5 0.8`
	`plot demo 101`
		`@pplane`
		`@hopf_locus 101`
		`@period_contour 101`
		`@period_contour 102`
			Plot type: `symbol`
			
			Label location: default
			Label location: default

2.7	`stability demo 2.2 0.8` `plot demo`	`@spectrum 1003`	Axes limits: default
2.8	`stability_loop demo` `plot demo 102`	`@pplane`	Plot type: `rcode`
2.9a	`plot demo 102`	`@spectrum 1002`	Axes limits: default
2.9b	`plot demo 102`	`@spectrum 1013`	Axes limits: default
2.10	`stability_boundary demo 102 1.75 0.3 1.75 0.7` `plot demo 102`	`@pplane` `@stability_boundary 101`	Plot type: `rcode`

2.11	`copy_hopf_loci demo 101 102`
	`copy_period_contours demo 101 102`
	`plot demo 102`
		`@pplane`
		`@hopf_locus 101`
		`@period_contour all`
		`@stability_boundary 101`
			Plot type: `symbol`
			
			Label locations: default

2.12	`set_worked_example_inputs 1`
	`new_pcode workedex`
	`hopf_locus workedex 101 -1 0 -1 6`
	`hopf_locus workedex 101 1 0 1 6`
	`plot workedex 101`
		`@pplane`
		`@hopf_locus 102`
			Plot type: `rcode`

Figure	Run commands	Plot commands	Plot options

2.13	`set_worked_example_inputs 7`
	`ptw_loop workedex`
	`hopf_locus workedex 102 1 0 1 6`
	`plot workedex 102`
		`@pplane`
		`@hopf_locus 102`
			Plot type: `rcode`

2.14	`plot workedex 102`	`@ptw 1037`	

2.17a	`set_worked_example_inputs 14`
	`stability_loop workedex`
	`plot workedex 103`
		`@spectrum 1008`	Axes limits: default

2.17b	`plot workedex 103`	`@spectrum 1008`	Axes limits: `-0.036 0.002 -0.05 0.4`

2.17c	`set_worked_example_inputs 16`
	`stability workedex -2.0 3.0`
	`plot workedex`
		`@spectrum 1022` (The rcode number will be depend on how many test runs were performed in earlier stages)	Axes limits: default

2.18	`plot workedex 103`	`@pplane`	Plot type: `rcode`

2.19	`stability_boundary workedex 103`
	`0.857 2.171 0.285 2.171`
	`stability_boundary workedex 103`
	`-0.857 2.171 -1.428 2.171`
	`plot workedex 103`
		`@pplane`
		`@stability_boundary all`
			Plot type: `symbol`

2.20	`set_worked_example_inputs 21`
	`stability_boundary workedex 103`
	`0.857 2.171 0.285 2.171`
	`stability_boundary workedex 103`
	`-0.857 2.171 -1.428 2.171`
	Note: the `stability_boundary` runs are not needed for this plot but are included here for consistency with the order in §2.3
	`plot workedex 103`
		`@pplane`	Plot type: `period`

Figure	Run commands	Plot commands	Plot options

2.21	`period_contour workedex 103 period=50`
	`-1.0 0.9 -0.2 0.9`
	`period_contour workedex 103 period=100`
	`0.85 1.6 0.85 2.2`
	`period_contour workedex 103 period=150`
	`0.9 2.2 0.2 2.2`
	`period_contour workedex 103 period=200`
	`1.0 2.6 -0.4 2.6`
	`set_worked_example_inputs 24`
	`hopf_locus workedex 103 1 0 1 6`
	`plot workedex 103`
		`@pplane`
		`@hopf_locus 101`
		`@stability_boundary 103`
		`@stability_boundary 104`
		`@period_contour all`
		
		`@pointsfile pde_stable.data 9`
		`@pointsfile pde_unstable.data 8`
			Plot type: `symbol`
			
			Label locations:
			`delta=-1.8 delta=1.55`

2.22	`new_pcode workedex`
	`copy_hopf_loci 103 104`
	`copy_period_contours 103 104`
	`copy_stability_boundaries 103 104`
	`plot workedex 104`
		`@pplane`
		`@hopf_locus 101`
		`@stability_boundary 103`
		`@stability_boundary 104`
		`@period_contour all`
		
		`@pointsfile pde_stable.data 9`
		`@pointsfile pde_unstable.data 8`
			
			Label locations:
			`delta=-1.8 delta=1.55`

3.1	`set_homoclinic demo 101 101`
	`plot demo 101`
		`@pplane`
		`@hopf_locus 101`
		`@period_contour all`
			Plot type: `symbol`
			
			Label location: default

3.2a	`bifurcation_diagram demo c=0.8` `plot demo`	`@bifurcation_diagram 101`	Vertical axis: norm Axes limits: default
3.2b	`bifurcation_diagram demo A=2.6` `plot demo`	`@bifurcation_diagram 102`	Vertical axis: period Axes limits: default

Figure	Run commands	Plot commands	Plot options

3.3a	`bifurcation_diagram demo c=0.6 variable=W`
	
	`plot demo`
		`@bifurcation_diagram 103`	Vertical axis:
			norm max min
			Axes limits: default

3.3b	`plot demo`	`@bifurcation_diagram 103`	Vertical axis: max mean stst Axes limits: default
3.4a	`ptw_loop demo1` `plot demo1 101`	`@pplane`	Plot type: `symbol`

3.4b	`hopf_locus demo1 101 1.065 21.0 1.08 21.0`
	`period_contour demo1 101 period=3000 1.085 20.0 1.08 20.0`
	`plot demo1 101`
		`@pplane`
		`@hopf_locus 101`
		`@period_contour 101`
			Plot type: `symbol`
			
			Label location: default

3.5	`bifurcation_diagram demo1 c=20.2` `plot demo1`	`@bifurcation_diagram 101`	Plot choice: norm Axes limits: default

3.6a	Change grid to 50×15 in `demo1/parameter_range.input`
	`ptw_loop demo1`
	`plot demo1 102`
		`@pplane`	Plot type: `symbol`

3.6b	Change `iwave` to 2 in `demo1/constants.input`
	`ptw_loop demo1`
	Reset `iwave` to 1 in `demo1/constants.input`
	Reset grid to 5×5 in `demo1/parameter_range.input`
	`plot demo1 103`
		`@pplane`	Plot type: `symbol`

3.7	Change `iwave` to 0 in `demo/constants.input`
	`ptw_loop demo`
	`copy_hopf_loci demo 101 103` (at warning: `y`)
	`copy_period_contours demo 101 103` (at warning: `y`)
	Reset `iwave` to 1 in `demo/constants.input`
	`plot demo 103`
		`@pplane`
		`@hopf_locus 101`
		`@period_contour all`
			Plot type: `symbol`
			
			Label location: default

Figure	Run commands	Plot commands	Plot options
3.12a	`stability_loop demo3` `plot demo3 101`	`@pplane`	Plot type: `rcode`

3.12b	`stability_boundary demo3 101`
	`8.21E-4 9.75 8.22E-4 9.75`
	`plot demo3 101`
		`@pplane`
		`@stability_boundary 101`
			Plot type: `symbol`

3.13a	`plot demo3 101`	`@spectrum 1003`	Axes limits: default
3.13b	`plot demo3 101`	`@spectrum 1002`	Axes limits: default

3.16	`plot demo 101`	`@pplane`
		`@hopf_locus 101`
		`@period_contour 101`
		
		`@period_contour 102`
			Plot type: `symbol`
			
			Label location:
			`c=0.8 c=0.5`
			Label location:
			`c=0.7 A=0.5 A=0.8 c=0.4`

3.17	`plot demo`	`@bifurcation_diagram 102`
		
		`@line 0.66 10.0 0.66 20.5`
		`@text 0.5 13.5 "Unstable"`
		`@text 0.9 13.5 "Stable"`
			Vertical axis: period
			Axes limits: default

References

E. Anderson, Z. Bai, C. Bischof, S. Blackford, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, D. Sorensen: LAPACK Users' Guide (Third ed.), Society for Industrial and Applied Mathematics, Philadelphia (1999).

F.V. Atkinson: Discrete and Continuous Boundary Problems, Academic Press, New York (1964).

C. de Boor, B. Swartz: Collocation approximation to eigenvalues of an ordinary differential equation: the principle of the thing. *Math. Comp.* **35**, 679-694 (1980).

G. Bordiougov, H. Engel: From trigger to phase waves and back again. *Physica D* **215**, 25-37 (2006).

F. Chatelin: The spectral approximation of linear operators with applications to the computation of eigenelements of differential and integral operators. *SIAM Rev.* **23**, 495-522 (1981).

E.J. Doedel, H.B. Keller, J.P. Kernévez: Numerical analysis and control of bifurcation problems: (I) Bifurcation in finite dimensions. *Int. J. Bifurcation Chaos* **1**, 493-520 (1991).

E.J. Doedel: AUTO, a program for the automatic bifurcation analysis of autonomous systems. *Cong. Numer.* **30**, 265-384 (1981).

J.J. Dongarra, J. Du Croz, S. Hammarling, R. J. Hanson: An extended set of FORTRAN basic linear algebra subprograms. *ACM Trans. Math. Soft.* **14**, 1-17 (1988a).

J.J. Dongarra, J. Du Croz, S. Hammarling, R.J. Hanson: Algorithm 656: an extended set of FORTRAN basic linear algebra subprograms. *ACM Trans. Math. Soft.* **14**, 18-32 (1988b).

J.J. Dongarra, J. Du Croz, I.S. Duff, S. Hammarling: A set of level 3 basic linear algebra subprograms. *ACM Trans. Math. Soft.* **16**, 1-17 (1990a).

J.J. Dongarra, J. Du Croz, I.S. Duff, S. Hammarling: Algorithm 679: a set of level 3 basic linear algebra subprograms. *ACM Trans. Math. Soft.* **16**, 18-28 (1990b).

B. Fornberg: Calculation of weights in finite difference formulas. *SIAM Rev.* **40**, 685-691 (1998).

C.A. Klausmeier: Regular and irregular patterns in semiarid vegetation. *Science* **284**, 1826-1828 (1999).

H.O. Kreiss: Difference approximation for boundary and eigenvalue problems for ordinary differential equations. *Math. Comp.* **26**, 605-624 (1972).

C.L. Lawson, R.J. Hanson, D. Kincaid, F.T. Krogh: Basic linear algebra subprograms for FORTRAN usage. *ACM Trans. Math. Soft.* **5**, 308-323 (1979).

J.J. Moré, K.E. Hillstrom, B.S. Garbow: The MINPACK project. In: Sources and Development of Mathematical Software, ed. W.J. Cowell, Prentice-Hall, pp. 88-111 (1984).

J.D.M. Rademacher, B. Sandstede, A. Scheel: Computing absolute and essential spectra using continuation. *Physica D* **229**, 166-183 (2007).

J.D.M. Rademacher, A. Scheel: Instabilities of wave trains and Turing patterns in large domains. *Int. J. Bifur. Chaos* **17**, 2679-2691 (2007).

J.A. Sherratt: Numerical continuation methods for studying periodic travelling wave (wavetrain) solutions of partial differential equations. Submitted (2011a).

J.A. Sherratt: Pattern solutions of the Klausmeier model for banded vegetation in semiarid environments II. Patterns with the largest possible propagation speeds. *Proc. R. Soc. Lond.* A in press (2011b).

J.A. Sherratt: Numerical continuation of boundaries in parameter space between stable and unstable periodic travelling wave (wavetrain) solutions of partial differential equations. Submitted (2011c).

J.A. Sherratt, M.J. Smith: Periodic travelling waves in cyclic populations: field studies and reaction-diffusion models. *J. R. Soc. Interface* **5**, 483-505 (2008).

B. Smith, J. Boyle, J. Dongarra, B. Garbow, Y. Ikebe, V. Klema, C. Moler: Matrix eigensystem routines, EISPACK guide. *Lecture Notes in Computer Science* **6**, Springer-Verlag, New York (1976).

M.J. Smith, J.A. Sherratt: The effects of unequal diffusion coefficients on periodic travelling waves in oscillatory reaction-diffusion systems. *Physica D* **236**, 90-103 (2007).