GETTING PRACTICE WITH AUTO2007 – OPERATING INSTRUCTIONS

Preliminary operations

a) Open the Min-GW shell by selecting from the Windows menu: **Programmi → MinGW → MinGW Shell**

b) on the MinGw-Shell, go to the directory where you put the files used in the case study:

c) *$ cd auto/07p/demos/bioreatt*

Remark

(remember that the slash character in Linux is " / " which is in the opposite direction with respect to the one " \ " used in theWindows-Dos environment)

d) Open with a text editor the file c.bioreatt in the path:
   C:\MinGW\msys\1.0\home\YOUR_USER_NAME\auto\07[\demos\bioreatt\bioreatt.c

The fundamental operations to be performed with AUTO are:

1. **run** the continuation program AUTO2007 (the shell command will be **@r**)

2. **save** the results of the continuation to an output file (with **@sv**) and/or **append** the results of the continuation to a preexisting file (**@ap**)

3. **represent** graphically the results (**@pp**)

Example 1:

γ **[PAR(2)] is held constant**

Da [PAR(1)] is decreasing from 2.5 to 0

The values adopted in the constants file c.bioreatt are discussed in detail in the presentation. The file c.bioreattor in the folder is at the beginning in its initial configuration. Run the following command from the shell:

@r bioreatt

The results of the continuation will be saved on three different files:

- *fort.7*

- *fort.8*

- *fort.9*

The file fort.7 contains the most concise report about the continuation just performed. The files fort.8 anf fort.9 are larger, with more detail on the computation.

The temporary fort.* files can be copied to another class of files (with extension *.bioreatt) by typing the command

@sv bioreatt

In this way the temporary files are moved to other three files:

- *fort.7 → p.bioreatt*

- *fort.8 → q.bioreatt*

- *fort.9 → d.bioreatt*

In general, by typing

@sv xxx

(where xxx is a generic string of characters) the temporary fiels are copied to three different files:
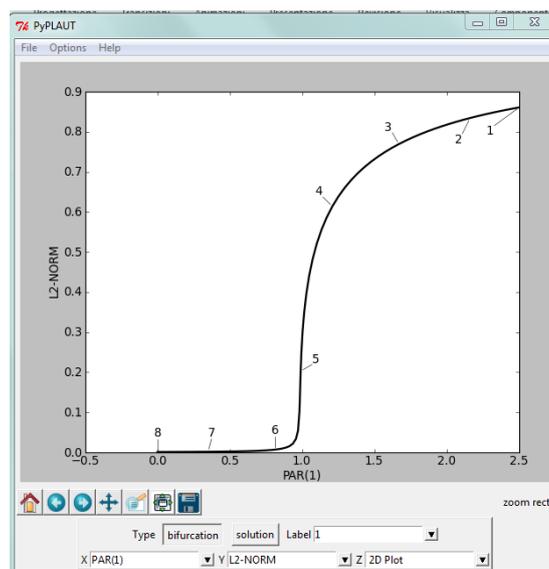
fort.7 → b.xxx

fort.8 → s.xxx

fort.9 → d.xxx

For the graphical representation one can use the executables provided by the installation of PyPlaut:

@pp bioreatt

A graphical window should appear:

The graph represents the Euclidean norm of the state variables with respect to the continuation parameter.

It is possible to change the variables illustrated by changing the inputs in the menu X and the menu Y. For example one can report the U(1) variable with respect to the continuation parameter by changing the variable in the Y-window:

L2-NORM → U(1)
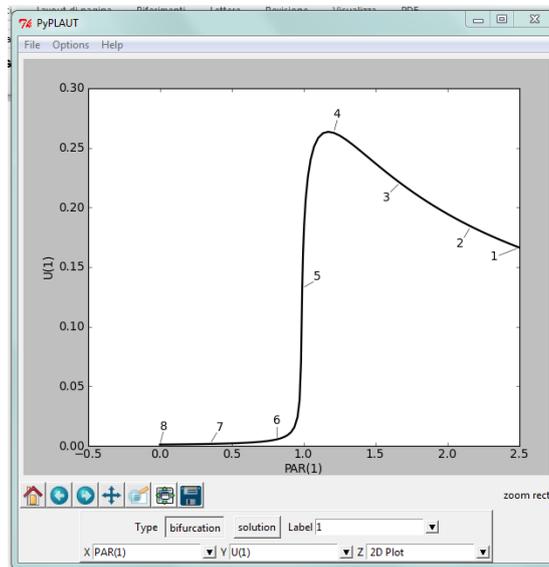
One can notice that:

a) *some points on the curve are marked with numbers, which correspond to the label points reported as output in the continuation: the point # 1 corresponds to the starting point of the continuation, the point #8 (EP) is the end point of the continuation (the lower limit PAR(1)=0 has been reached).*

b) *the curve is, for the moment a unique, black, solid line*

*To run other examples on the MinGW shell, you should the graph window by selecting **File → Quit**. With this operation, the Min-GW shell is made again available.*

Example 2:

Continuation 1

Da [PAR(1)] is held constant

γ [PAR(2)] varies from 0.9 to 0.6 (decreasing γ)

The file can be opened and edited with a common text editor (wordpad, notepad, notepad++). Constants to be changed in the file c.bioreatt.

ICP → [2]

UZR → {2: [0.60]}

We are still moving from the initial point (Da = 2.5, γ = 0.9), thus IRS is still 0.

Be aware to save the c.bioreatt file after you have completed the changes!!

Once the c.bioreatt file is modified and saved, it is possible to execute once more the continuation program.

@r bioreatt

The results of the continuation can be again saved in the files b.bioreatt, d.bioreatt, s.bioreatt

@sv bioreatt

It is possible a graphical representation of the continuation by typing:

@pp bioreatt

Continuation 2

Da [PAR(1)] decreases from 2.5 to 0.0

γ [PAR(2)] is held constant

Constants to be changed in the file c.bioreatt.

ICP(1) $\rightarrow$ [1]

IRS $\rightarrow$ 2 new label corresponding to PAR(2) = 0.6.

Remark:

When IRS ≠ 0, the software will search the starting value from the previous computations stored in the files *.bioreatt (or, in general, *.xxx). If you do not save (or the IRS value to be recalled is absent in the bioreatt files) the code will generate an error message

Again, one can run (and save) the continuation of the model at γ = 0.6 with the traditional commands:

@r bioreatt

@sv bioreatt

Remark:

The execution of @sv will delete **all** the computations previously accomplished with AUTO and stored in the bioreatt files. Be careful to use the command: you are losing all the information concerning the previous steps of your continuation.

For the graphical representation:

@pp bioreatt

It should be noted that the results are qualitatively different: the stable stationary solutions are still reported with the solid black lines, but one can observe the appearance of an unstable stationary solutions branch which is reported with the dashed line.
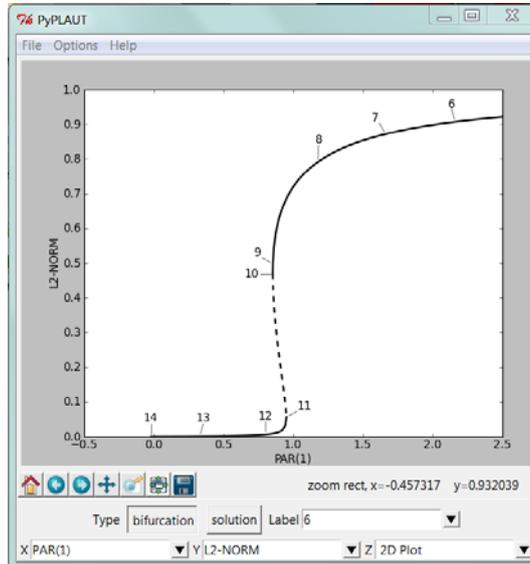
Continuation 3 (Two parameter continuation of the Limit Point bifurcations)

Da [PAR(1)] and γ [PAR(2)] will change together

a.   Forward continuation (that is, with a positive stepsize DS):

IRS → 11	(IT MUST BE a label corresponding to a bifurcation point)
ICP → [1,2]	(the continuation is with respect to two parameters: PAR(1) and PAR(2))
ISW → 2	
DS → +0.01	(*forward* continuation)
NMX → 80	
NPR → 20	

The last two modifications are not crucial. They are (warmly) suggested for the problem under investigation.

Now one can run AUTO:

@r bioreatt

After the two parameter continuation has been accomplished, it is better to save the results of the computation with a different name: this can avoid to delete the starting point for the backward continuation that has been stored in the bioreatt file. For example, one can type:

@sv bioreatt2P

Now, in the folder there should be:

  i)   *the results of the previous continuation with extension *.bioreatt*

  ii) *the results of the current continuation with extension *.bioreatt2P*

The availability of the results of the previous continuation is really useful for the subsequent "backward" 2 parameter continuation
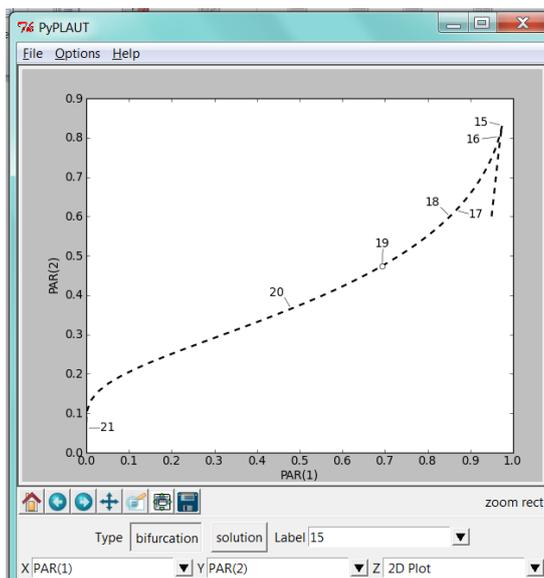
For the graphical representation type:

@pp bioreatt2P

The following window will appear:
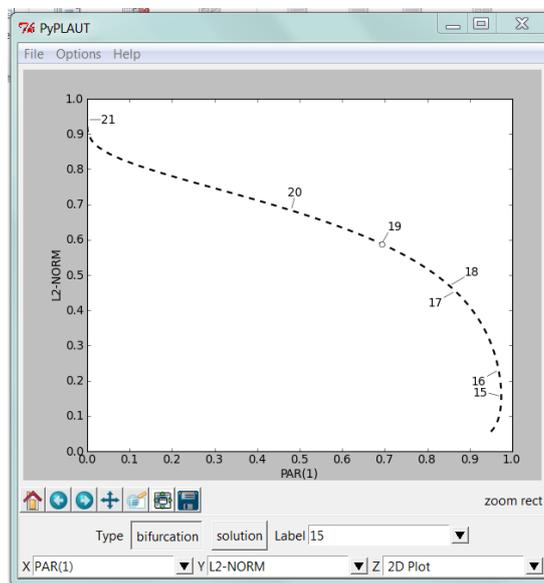
*In order to have a useful bidimensional representation it is suggested to leave PAR(1) as the x-variable and change the y-variable in the graph **L2-NORM → PAR(2)** (leave always the 2D plot option)*

b.   Backward continuation (that is, with a negative stepsize DS)

There is only a change to perform with respect to the previous continuation

DS → -0.01

It should be remarked that the continuation restarts from the label 11 which has not been deleted in the previous steps (the files have not been overwritten) and it is still in the bioreatt files
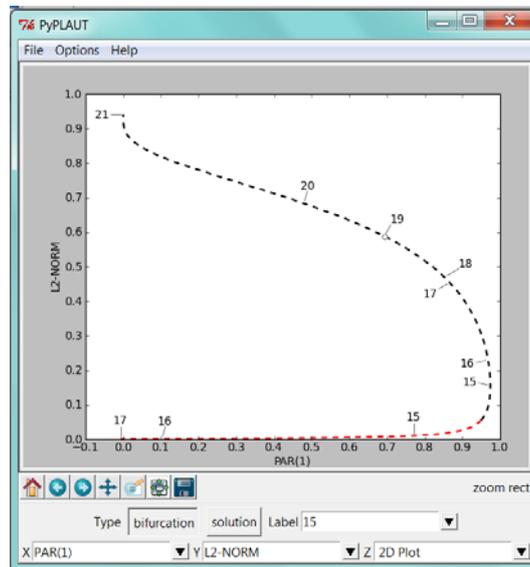
*One can still run AUTO:*

@r bioreatt

The results of the continuation can be now APPENDED (that is added to the files without deleting previous information) on the 2-parameters continuation file previously created

@ap bioreatt2P

Then a graphical representation is possible:

And choosing PAR(1) as the x-variable and PAR(2) as the y-variable one can eventually end up with the following figure:
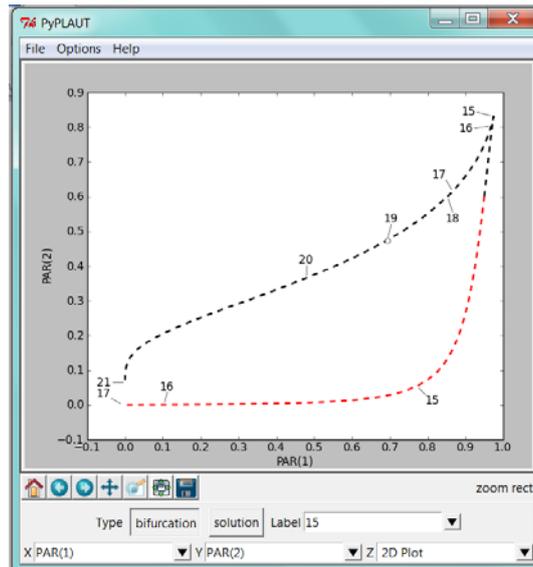
Example 3

Continuation 1

> *Da [PAR(1)] is held constant*
>
> γ *[PAR(2)] varies from 0.9 to 0.52 (γ is decreasing)*

Constants to be changed in the file c.bioreatt.

We come back to starting stationary solution, therefore we should retrieve the constant values related to the first continuation:

IRS	$\rightarrow 0$
ICP	$\rightarrow [2]$
ISW	$\rightarrow 1$
UZR $\rightarrow \{2: [0.52]\}$	

The only differenze is the UZ value (γ = 0.52)

Once the c.bioreatt has been modified, it is possible to run the continuation program.

@r bioreatt

and then save the results on the bioreatt files:

@sv bioreatt

Continuation 2

Constants to be changed in c.bioreatt.

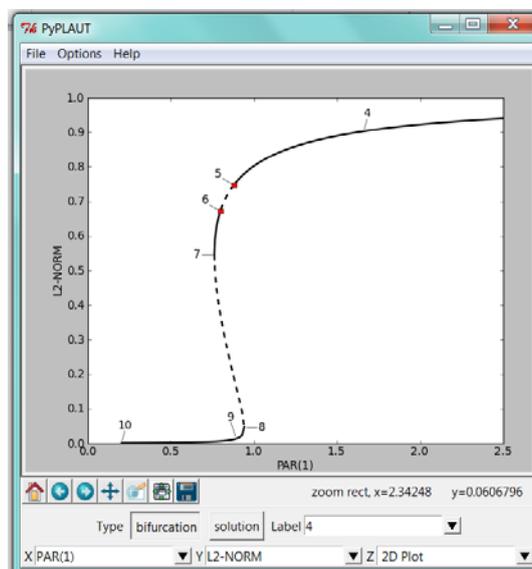|	
ICP	→ [1]
IRS	→ 2 – new label corresponding to PAR(2) = 0.52.

Again, we can run (and save) the continuation with respect to Da (with fixed γ = 0.52), starting from the label corresponding to γ=0.52, by executing the commands:

@r bioreatt

@sv bioreatt

For the graphical representation:

@pp bioreatt

In this case there are two lines of unstable stationary solutions, represented with the dashed line. The Hopf Bifurcations (HB points) are reported with red circles in the graph.

Continuation 3 (Continuation of the periodic solutions from the Hopf bifurcation)

Constants to be changed in c.bioreatt.

|	
IPS	→ 2
ICP	→ [1,11]
ISP	→ 2
IRS	→ 5 (or, alternatively, 6)

And then execute AUTO:

@r bioreatt

Now, it could be proper to append the results of the current continuation to the previous one, in order to have a complete representation of all the solutions found

@ap bioreatt

It is possible to show graphically the results. Choosing PAR(1) as the x-variable and MAX U(1) as the y-variable one can eventually end up with the following figure, where the maximum attained by the oscillations is reported with a red solid line:
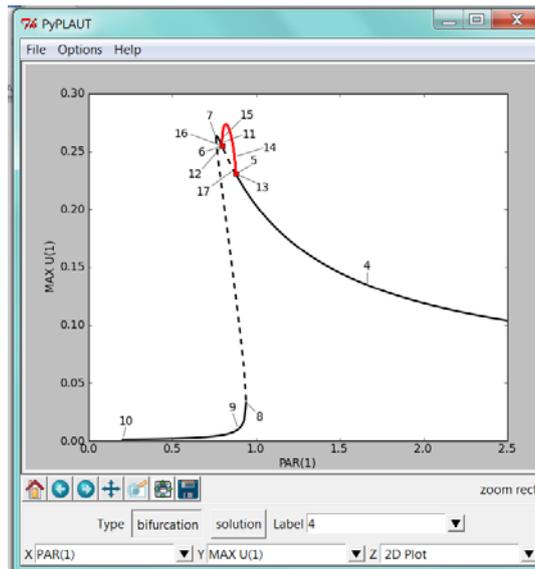
Continuation 4 (Two parameter continuation of the Hopf bifurcations)

Da [PAR(1)] and γ [PAR(2)] will change together

Constants to be changed in c.bioreatt.

IPS	→ 1
ICP	→ [1,2]
ISP	→ 1
ISW	→ 2
DS	→ -0.01
IRS	→ 5 (this must be a bifurcation point)
NMX	→ 160 (suggested for the current continuation)

After the execution of AUTO:

@r bioreatt

It is preferable to append the results in the file already implemented for the two parameters continuation:

@ap bioreatt2P

In an analogous way one can accomplish the "forward" 2-parameter continuation, changing the DS constant in c.bioreatt:

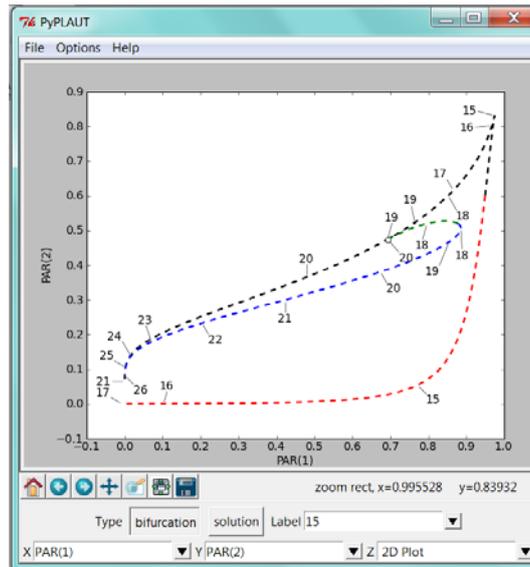|	
DS	→ +0.01

Execute AUTO:

@r bioreatt

Then, append the computation results in the file bioreatt2P

@ap bioreatt2P

The results of the 2 parameter continuation (both limit points and Hopf bifurcations) can be graphically reported:

Example 4 – Optimization problem

Constants to be changed in c.bioreatt.

|		
IRS	→ 0	
IPS	→ 5	*(IPS value for the detection of extrema of)*
ICP	→ [10,1,4]	*(maximum of the function with respect to 2 parameters, PAR(1) and PAR(4), the objective function, PAR(10), is treated by AUTO as an additional parameter)*
ISW	→ 1	*(continuation with respect to one parameter)*
DS	→ +0.01	
UZR	→ {}	
NMX	→ 80	

Traditional run of the continuation software

@r bioreatt

An extremum of the objective function should be detected as PAR(1) is varying (notice that PAR(4) is constant) at label 3. One can save the results:

@sv bioreatt

Representing graphically (Choosing FOPT as the x-variable and PAR(1) as the y-variable) one can appreciate that the maximum of the objective function with respect to Da may be, in fact, regarded as a limit point when FOPT is considered as an additional parameter:
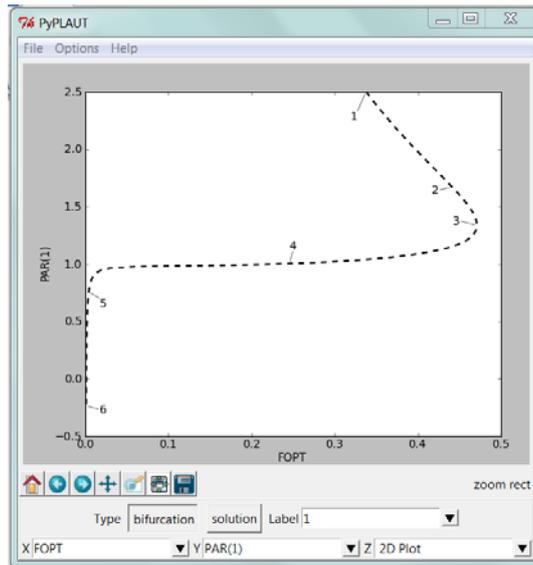
Then, a two parameter continuation (with respect to PAR(1) and PAR(4)) is accomplished by performing a continuation of the LP detected at label 3:

IRS → 3 (label related to the LP point detected in the previous continuation)

There are no further changes to accomplish in c.bioreatt. Execute AUTO:

@r bioreatt

The LP observed in the actual continuation represents the maximum of the objective function with respect to the parameters Da and γ.

One can append the last results to the previous continuation:

@ap bioreatt

And take a look at the results reported in a 3D graph (PAR(1) as the x-variable, PAR(1) as the y-variable, FOPT as the z-variable):

@pp bioreatt