Motivations

- Given a parameterized, autonomous, nonlinear, dynamical system of the form:

\[
\frac{dx}{dt} = f(x, \theta), \quad x, f \in \mathbb{R}^n, \quad \theta \in \mathbb{R}^m
\]

- The goal is to compute the asymptotic solutions \(x(t)_{t \to \infty}\) changes as \(\theta\) varies.
Motivations - Example

- A Continuous Stirred Tank BioReactor (CSTBR) is considered.
- Assumptions:
  - Perfect mixing (homogenous concentrations in the system)
  - Continuously fed with a substrate S
  - The tank volume V and the feed F are constant:

- The species are modeled with an unstructured model: biomass X in the reactor reacts with a substrate S to give a product P

Motivations - Example

- System dynamics is governed by the mass balance equations for the biomass X and the substrate S (x = [X, S] ∈ R^2)

\[
\begin{align*}
    \frac{dX}{dt} &= \frac{F}{V} X_F - \frac{F}{V} X + \mu(S) X - \sigma(S) X \\
    \frac{dS}{dt} &= \frac{F}{V} S_F - \frac{F}{V} S - \sigma(S) X
\end{align*}
\]

For the case at hand:

\[
\begin{align*}
    \text{ACC} &= \text{IN} - \text{OUT} + \text{GEN}
\end{align*}
\]
Motivations - Example

- Equations in **dimensionless** form:

  \[
  \frac{dx_1}{d\tau} = x_{1F} - x_1 + Da \, M(x_2) \, x_1 \\
  \frac{dx_2}{d\tau} = -x_2 + Da \, \Sigma(x_2) \, x_1
  \]

  **Dimensionless state variables:**

  \[
  x_1 = \frac{X}{Y(S_F)S_F} \\
  x_2 = \frac{S_F - S}{S_F} \\
  \tau = \frac{t}{V/F}
  \]

  **Dimensionless parameters:**

  \[
  Da = \frac{\mu(S_F)}{F/V} \\
  \Sigma = \frac{\sigma(S)}{\sigma(S_F)} \\
  x_{1F} = \frac{X_F}{Y(S_F)S_F} \\
  M = \frac{\mu(S)}{\mu(S_F)}
  \]

Motivations - Example

- \( \mu(S) \): Biomass growth rate
- \( \sigma(S) \): Substrate consumption rate

- Many expressions in the literature. We will refer to the ones used by Agrawal et al. (Chem. Eng. Sci., 1981, 37(3), 453-462)

  \[
  M(x_2) = (1 - x_2) \exp\left(\frac{x_2}{\gamma}\right) \\
  \Sigma(x_2) = M(x_2) \frac{1 + \beta}{1 + \beta - x_2}
  \]
Motivations - Example

- The dimensionless model thus involves two state variables
  \[ x = \begin{bmatrix} x_1, x_2 \end{bmatrix} \quad x \in \mathbb{R}^2 \]

  and four parameters:
  \[ \theta = \begin{bmatrix} Da, \gamma, \beta, x_{1F} \end{bmatrix} \quad \theta \in \mathbb{R}^4 \]

GOAL:

- To analyze the quantitative and qualitative changes of the regime solutions of the state variables \( x \) as the \( \theta \) parameters vary.
- A first possibility is the numerical integration of the model for a wide range of parameter values and initial condition

  "BRUTE FORCE" APPROACH

Example – Model investigated with a "brute force" approach

- \( Da = 0.6 \) (\( \beta = 0.05, \gamma = 0.52, X_{1F}=0.001 \))

- The system evolves towards a unique steady state asymptotic stationary solution for any initial condition:
  - biomass tends to disappear and the substrate concentration is nearly equal to the feed substrate concentration
Example – Model investigated with a “brute force” approach

- \( Da = 0.77 \) (\( \beta = 0.05, \gamma = 0.52, X_{1F} = 0.001 \))

- **Multiplicity** of stable stationary solutions is observed
  - The asymptotic steady behaviour depends on the initial condition

---

Example – Model investigated with a “brute force” approach

- \( Da = 0.8 \) (\( \beta = 0.05, \gamma = 0.52, X_{1F} = 0.001 \))

- **Multiplicity** of regime solutions is observed (a stationary and a periodic solution)
  - The asymptotic behaviour depends again on the initial condition
Example – Model investigated with a “brute force” approach

- **Da = 1.5** \((\beta = 0.05, \gamma = 0.52, X_{1F} = 0.001)\)

![Graphs showing the evolution of the system over time](image)

- The system evolves towards a **unique** steady state asymptotic **stationary** solution for any choice of the initial condition
  - This solution is characterized by high conversions

Example – Model investigated with a “brute force” approach

- The evaluation of the changes of the asymptotic solution as parameters vary via **direct numerical simulation** may require **time**

![Graphs showing the impact of parameters on the solution](image)
Why a continuation algorithm?

- Roughly speaking ...
- Given the (stationary) solution $x_s(\lambda_0)$ at $\lambda = \lambda_0$ of the model $f(x, \lambda) = 0$
- the goal is to estimate the new stationary point at $\lambda = \lambda_0 + \Delta \lambda$ starting from the older one.
- Continuation algorithms aim to trace the loci of the solutions of algebraic equations (and also periodic solutions) given a first tentative value.
- The Continuation Algorithm used is AUTO

Why AUTO?

- AUTO is a software for continuation and bifurcation problems in ordinary differential equations
- Cited in **more than 1500** contributions on scientific journals (as referred by Scirus and Scholar)
Why AUTO?

- Tested even on high order systems of ODEs (~ 150-200).
- Easy to configure and run on Unix/Linux environments
  - Things get more complicated with the Windows OS.
- It is not a commercial software, hence user documentation, examples, and customer support is lacking.

A brief history of AUTO

- The historical evolution in the development of AUTO:
  - The first version was distributed in 1980
  - AUTO86 (1986): written in Fortran77 and intended for operation from command line.
  - AUTO94 (1994): parallel version
  - AUTO97 provides a Graphical User Interface, although rather limited. Allows more operations than AUTO86. Still in Fortran77
  - AUTO2000: it is written in C and includes revised command line interface and possibility of controlling the program execution via PYTHON scripts.
  - AUTO2007: similar to AUTO2000 but it is written in Fortran90
Basic notions

- AUTO2007 is constituted by a series of programs in Fortran 90, that are arranged in a series of subdirectories.

![Diagram]

**Basic notions – User supplied files**

- The directory AUTO2007/demos contains a series of folders each of them pertaining a different illustrative case study relative a specific model.
- For each model **xxx**, two files may be modified by the user:
  - **The Equations-File xxx.f90**
    - A Fortran90 file where the user will write the **mathematical model** to be investigated
  - **The Constants-File c.xxx**
    - A text file containing the **numerical parameters** used for each continuation
- These are the **only** files to be modified during the computation
**User supplied files – File xxx.f90**

- The **mathematical model** is written in the file `bioreatt.f90`
  - It is constituted by different Fortran **subroutines**.
  - Two subroutine are of interest for the parameter continuation of the steady state solutions:

- **SUBROUTINE** `FUNC`
  - In this subroutine one defines the mathematical model (that is, the **FUNCTION** representing the right hand side). It is also possible to define the Jacobian matrix of the ODEs set.

- **SUBROUTINE** `STPNT`
  - The starting point for the continuation are here reported (**STarting PoINT**)  

**User supplied files – File xxx.f90**

- The state variables are defined as components of the **U vector**
  - U(1) -> $x_1$
  - U(2) -> $x_2$

- Parameters are defined as components of the **PAR vector**
  - PAR(1) -> Da 
  - PAR(2) -> $\gamma$ 
  - PAR(3) -> $\beta$ 
  - PAR(4) -> $X_{IF}$

- **AUTO** allows to study a model **up to a maximum of 9 parameters**. The components PAR(10) and PAR(11) are parameters managed by AUTO:
  - PAR(10): an objective function to be eventually taken into account
  - PAR(11): period pertaining the periodic solutions
User supplied files – File xxx.f90

- In the file there are also other subroutines:

  - SUBROUTINE BCND
    - To be used when dealing with boundary conditions problems

  - SUBROUTINE ICND
    - Definition of Integral CoNDitions

  - SUBROUTINE FOPT
    - Definition of objective functions

  - SUBROUTINE PVLS
    - Definition of solution measures

These subroutines are not needed at the moment: They can be also left unfilled

User supplied files – File c.xxx

- After the file file xxx.f90 is written, it will be **no longer** modified during the continuation.
- Hereafter, the user will manage **only** the constants-file c.xxx for all the simulations
AUTO2007 – File c.xxx
Constants of common use

- **NDIM**
  - Dimension of the system of ODEs (equivalently, the Number of state variables). This constant is constant during all the simulations.
    - ODEs are defined in the subroutine FUNC in the file xxx.f90.

- **IPS**
  - Integer type variable. This constant defines the problem type:
    - Continuation of stationary solutions of ODEs: IPS = 1.
    - Computation of periodic solutions: IPS = 2.
    - Algebraic optimization problem: IPS = 5.
  - For further problem types and more details, refer to the AUTO2007 guide

- **IRS**
  - Sets the label of the solution where the computation is to be restarted
  - IRS = 0: typically used in the first run of a new problem. A starting solution must be defined in the user-supplied routine STPNT.
  - IRS > 0: Restart the computation at the previously computed solution with label IRS.

- **ILP**
  - Boolean variable.
    - ILP = 0 No detection of limit points in the continuation.
    - ILP = 1 Limit points detection.
  - The concept of Limit point will be discussed in the following.
AUTO2007 – File c.xxx
Constants of common use

- **ICP**
  - Array of the free parameters used for the continuation.
  - The parameter that appears first in the ICP list is called the “principal continuation parameter”.

- **NMX**:
  - The maximum number of steps to be taken along any solution branch.

- **DS**
  - Real number. This constant defines stepsize to be used for the first attempted step along the solution branch. DS may be chosen positive or negative: changing its sign reverses the direction of the computation.

- **DSMIN, DSMAX**
  - Real numbers (positive). They represent respectively the minimum and the maximum absolute values allowable for the stepsize.
  - The choice of the optimal values for DMIN and DSMAX is highly problem-dependent.
AUTO2007 – File c.xxx
Constants of common use

- **ISW**
  - Integer number.
  - ISW = 1: normal continuation
  - ISW = 2: two parameters continuation
  - ISW = -1: for more complicated situations.
    - To be used when a so-called “branch-switching” is required

- **UZR**
  - Allows the setting of parameter values at which the corresponding solutions can be labeled
  - UZR = {}: no solution labelling is needed.

AUTO2007 – File c.xxx
Constants of occasional use

- Other variables:
  - **JAC**
    - Indicates whether derivatives are supplied or not by the user
    - JAC = 0: no derivatives are given by the user. They are obtained by differencing
    - JAC = 1: derivatives with respect to the state variables and parameters are given in the user-supplied routine FUNC.

    - In most of the cases, the evaluation of the derivatives is not necessary (JAC=0 works as well). It may be however useful for sensitive problems and for computations of extended systems.
**Constants of occasional use**

- The following variables are not used frequently in the computations.
  - **RL0, RL1**
    - Real numbers. They represent, respectively, the lower and the upper bound of the principal continuation parameter. For the case at hand one can choose $RL0=0.0$ (we are not interested in solutions at $Da < 0$) and $RL1=2.5$ (the algorithm will stop when $Da > 2.5$)
  - **A0, A1**
    - Positive, real numbers. They represent, respectively, the lower and the upper bound of a principal solution measure.
    - They are seldom used. It is suggested to give the values $A0 = 0$ and $A1$ equal to a large number.

**Constants for skilled users**

- Seldom required to be modified. Read carefully the AUTO2007 guide before to change them. The predefined values are often adequate for most of the problems.
  - **IAD**
    - Integer number. Adapt the mesh every IAD steps along the continuation branch. Strongly recommended value: $IAD = 3$
  - **EPSL, EPSU, EPSS**
    - Real numbers. Relative convergence criterions for the iterations of the predictor/corrector method. Suggested by the authors
      Recommended values: $EPSL = EPSU \approx 10^{-6} \sim 10^{-7}$ e $EPSS \sim 1000$
  - **ITMX, NWTN, ITNW**
    - Integer numbers. Maximum number of iterations
      Recommended values: $ITMX = 8$, $NWTN = 3$, $ITNW = 5$. 
AUTO2007 – File c.xxx
Constants for (really) skilled users

- IPLT
  - Integer number. Gives the choice of the principal solution measure:
    the second real number written per output line
    - IPLT = 0: Euclidean norm of the state variables (choice usually
      adopted)

- For a detailed description of all the numerical constants that can be
  modified one can refer to the AUTO2007 user guide
Goal:
Trace the stationary solutions of the model as the Damkohler number, \( Da \), varies (the other parameters are held constant):
- \( \gamma = 0.9 \)
- \( \beta = 0.05 \)
- \( x_{1F} = 0.001 \)

One is interested to the locus of the points
\[ x_s = x_s(Da) \]

Starting from the solution as it was computed at \( Da = 2.5 \), that is:
\[ x_{1S} = 0.166333 \]
\[ x_{2S} = 0.844414 \]

The following constants will not change the values for all the continuations performed
- \( NDIM = 2 \) (order of the ODEs)
- \( IPS = 1 \): Continuation of stationary solutions
- \( ILP = 1 \) (limit point detection)
- \( NTST = 50 \) (number of mesh intervals)
- \( NCOL = 4 \) (number of collocation points)
- \( IAD = 3 \)
- \( IPLT = 0 \)
- \( NBC = 0, NINT = 0 \)
- \( MXBF = 10, ITMX = 8 \)
• Constants depending on the specific run. They can change values in the following continuations
  - **IRS = 0 Important!!** Since this is the first continuation one should specify the starting point in the subroutine STPNT
  - **ICP = [1]** the principal parameter continuation is Da = PAR[1]
  - **UZR = {}** (we are not interested to label a specific solution for a given parameter value)
  - **DS = -0.01** starting point is at Da = 2.5 and we are interested at lower values: **DS < 0!!**
  - **DSMIN = 0.005, DSMAX = 0.05.** Empirical values.
  - **RLO = 0.0, RL1 = 10.0** lower and upper bound chosen for the current continuation: we are not interested on unphysical parameter values (Da>0).
  - **NMX = 100, NPR = 10**

---

**AUTO 2007 – First run: Example #1**

• A reasonable implementation for the file c.bioreatt could be

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**AUTO 2007 – First run: Example #1**

• In order to execute AUTO 2007 you should type on the linux shell, (in the directory where the AUTO file were copied) the command:
  - [@r bioreatt]
**AUTO 2007 – First run: Results**

- The results of the continuation are saved on the temporary files:
  - fort.7
  - fort.8
  - fort.9

- The results can be saved on a definitive file by typing:
  @sv bioreatt

- The file fort.7, fort.8 e fort.9 will be copied with the “bioreatt” extension:
  - fort.7 → b.bioreatt
  - fort.8 → s.bioreatt
  - fort.9 → d.bioreatt
AUTO 2007 – First run: Results – Solution diagram

- The results can be plotted on a solution diagram

\[
\begin{align*}
\text{PAR}(2) &= \gamma = 0.9 \\
\text{PAR}(3) &= \beta = 0.05 \\
\text{PAR}(4) &= X_1F = 0.001
\end{align*}
\]

Labels 1 and 8 are the begin and the end of the continuation

- Comments:
  - Only one stable steady state solution is asymptotically reached for any initial condition.
  - This scenario does not change with Da.

\[
\begin{align*}
\text{Da} &= 0.5 \\
\text{Da} &= 1.5
\end{align*}
\]
AUTO 2007 – Further computations: Example 2

- Continuations can be also performed for other $\gamma$ values
- For example, one can be interested at the stationary solution $x_\gamma(x)(D\alpha)$ for another value of the inhibition rate $\gamma$ e.g. $\gamma = 0.60$ (PAR(2) in the file bioreatt.f90).
- In this case one can perform two continuations with respect two different parameters

1. Continuation of the stationary solution with $D\alpha$ held constant and $\gamma$ moving from 0.9 to 0.6
2. Continuation starting from the solution obtained at $\gamma = 0.6$. The parameter $\gamma$ is held constant and $D\alpha$ decreases

AUTO 2007 – Example 2 – Continuation #1
How to modify the file c.bioreatt

- The continuation must performed with respect to the parameter $\gamma$ (PAR(2)) whereas $D\alpha$ is held constant (PAR(1))
  - IRS = 0: we are still starting from the stationary solution computed at $D\alpha = 2.5$ and $\gamma = 0.9$
  - ICP = [2]: the continuation is performed with respect to the parameter PAR(2) = $\gamma$
  - DS = - 0.01
  - UZR = {2: [0.60]}
- Motivation: to mark with a label the continuation point corresponding to $\gamma = 0.60$.
  - There are no other changes to be accomplished in the c.bioreatt file
How the file c.bioreatt has been modified

New parameter chosen for the continuation

The step is still negative!
Parameter γ should decrease

UZR = {2: [0.60]}
With this instruction it is required to mark with a label the solution point corresponding to PAR(2) = 0.60

AUTO 2007 – Example 2
Continuation #1: Results

Branch number
BR = 1

MX point:
It means abnormal termination of the computation

Types of the solution points
Now there is also the required UZ label corresponding to γ = 0.6

Label numbers
The UZ point is marked with the label 2
AUTO 2007 – Example Continuation #1: Results

- The continuation results can be again saved (@sv bioreatt.f) and plotted.

The point marked with label 2 is the starting point for the subsequent continuation.
It represents the stationary solution corresponding to Da=2.5 and γ=0.6.

AUTO 2007 – Example 2 – Continuation #2 How to modify the file c.bioreatt

- In the second step, the continuation has to be performed with respect to the parameter Da (PAR(1)) and γ is held constant (PAR(2) = 0.60).
  - IRS = 2: the continuation starts from the point corresponding to γ = 0.60 and Da = 2.5, which has been marked during the continuation #1.
  - ICP = [1]: the continuation has to be performed with respect to PAR(1) = Da.
  - DS = -0.01
  - No further changes in the file.

- IMPORTANT!
  - Execute the program only after the previous computations have been saved with the @sv command: the new starting value for the continuation must be stored in the files *.bioreatt.
AUTO 2007 – Example 2 – Continuation #1
How the file c.bioreatt has been modified

IMPORTANT!!
New starting point for the continuation

Parameter to be continued
PAR(1)

Negative step

AUTO 2007 – Example 2
Continuation #2: Results

• SOMETHING NEW IN THE OUTPUT!!

The label LP means Limit Point bifurcation
The results can be graphically represented

The continuation algorithm shows a **turning** in the opposite direction at $Da \sim 0.85$.

The branch becomes **unstable**. Such **qualitative** change of the solution is a **LIMIT POINT BIFURCATION**.

When $Da \sim 0.95$ another limit point bifurcation is observed, and the solution returns stable as $Da$ decreases.

In the range $Da = [0.85, 0.95]$ a **MULTISTABILITY** of Stable Steady State Solutions is observed.

When $Da = 0.9$ the solution regime does depend on the initial conditions.
**AUTO 2007 – Example 2**

One parameter continuation - Summary

- Graphical representation of the continuations performed

![Graphical representation](image)

**Some considerations - Summary**

- **Some clues:**
  - AUTO allows to investigate the model behavior for every parameter value combination by performing the correct sequences of variations of the parameters
  - Follow carefully the correct paths! (before getting lost following "wrong" parameter values)
**AUTO 2007 – Example 2**

**Some considerations**

- It was found that the occurrence of bifurcations in the model depends on the $\gamma$ value.
- Thus, one should be interested to find the points in the $(\gamma, Da)$ parameter plane corresponding to the bifurcations.
- This is possible by performing a **two-parameters continuation** of the limit points.

**AUTO2007 – Two parameter continuation**

- Once the last continuation has been saved it is possible to perform a **two parameter continuation**.
- Some stuff to be changed in the file c.bioreatt:
  - **IRS = 11**: in order to evaluate the locus of the bifurcation points as $Da$ and $\gamma$ vary, one must start from the label corresponding to the bifurcation point detected at $\gamma = 0.6$ (It should be however reminded that one can use also the other bifurcation point detected in the previous computation i.e. IRS = 10)
  - **ISW = 2**: the new assignment allows to compute a branch of bifurcation points in a two parameters space.
  - **ICP = [1,2]** the parameters free to change along the current continuation: the limit point bifurcations are evaluated in the $(Da, \gamma)$ plane. (N.B. The other parameters are held constant and equal to the initial values $x_{1f} = 0.01$ and $\beta = 0.05$)
    - **DS = +0.01**
AUTO2007 – Two parameter continuation

- Other constant to be changed (not fundamental, but strongly suggested for the current continuation)
  - $NMX = 80$
  - $NPR = 20$

AUTO2007 – Two parameter continuation

- A plausible form for the c.bioreatt file

New starting point for the two-parameter continuation
The label must be a bifurcation point

ICP = [1, 2]
Two parameters free to change along the continuation

ISW = 2
Two parameter continuation
**AUTO2007 – Two parameter continuation**  
**Results**

- Bifurcation diagram in the Da-$\gamma$ plane

Parameters PAR(1) and PAR(2) are varying together.

Two new labels:
- **CP**: Cuspid Point
- **BT**: Bogdanov-Takens point

Starting point for the two parameters continuation

Point #15
- Cuspid point

Point #19
- Bogdanov-Takens point
AUTO2007 – Two parameter continuation Results

- Starting from the same label IRS = 11 and giving a negative stepsize, one can compute the remaining part of the bifurcation curve:
  - DS = -0.01

Limit points bifurcation diagram
The closed curve borders the region in the parameters space characterized by steady states multiplicity.

No further information about their stability can be established.
**AUTO2007 – Exercise**

- Perform a continuation with respect to the Da parameter when $\gamma = 0.52$ (the other parameters are always $x1f = 0.001$ and $\beta = 0.05$)

- Constants to be changed for the continuation #1:
  - IRS = 0
  - ICP = [2]
  - ISW = 1
  - UZR = {2: [0.52]}

- Constants to be changed for the continuation #2:
  - ICP = [1]
  - IRS = number corresponding to the UZ label computed in the first continuation

**AUTO2007 – Exercise: Results**

A new bifurcation labelled with the string HB is encountered (Hopf Bifurcation). The Hopf bifurcation marks the onset of oscillatory regimes (limit cycles): the steady state solution is no longer stable and periodic regime solutions are observed.
**AUTO2007 – Exercise: Results**

- Results of the continuation

No stable steady states are observed in the parameter window between the HB points. The detection of Hopf bifurcations might suggest the occurrence of periodic stable solutions.

**AUTO2007 – Continuation of the periodic solutions**

- AUTO can also perform a continuation of the periodic solutions emerging from the Hopf bifurcation.
- Constants to be changed in the c.bioreatt file:
  - **Research of the periodic solutions** is performed by setting **IPS=2**
  - **ICP=[1,11]** (PAR(11) is an additional parameter introduced by AUTO representing the period of the regime solution: the continuation of the periodic solutions can be seen as a particular case of a two parameter continuation).
  - **ISP=2** (It allows to detect the stability of the periodic solution through computation of the Floquet multipliers).
  - **IRS**: number of the HB label corresponding to the Hopf bifurcation.
N.B. The computation of the continuation branch reaches the other HB bifurcation and it "comes back". This feature leads to the detection of spurious Limit Points.

The maximum value attained by the oscillation is displayed.

Solution diagram with respect to Da (with $\gamma = 0.5$)

- A multistability of solutions is again observed at intermediate Da values.
Two parameter continuation of the Hopf bifurcations

- It is possible to compute the loci of the Hopf bifurcations in the \((Da, \gamma)\) parameters space.
- The procedure is analogous to the one implemented for the Limit Point bifurcations. Again, one should start from the label of a bifurcation point.
  - **IRS** -> number corresponding to the HB label corresponding to the Hopf bifurcation.
- The setting of the other constants in the c.bioreatt file is the same of the Limit Points two-parameters continuation.
  - **ISW** = 2:
  - **ICP** = [1,2]
  - **DS** = ±0.01
  - **NMX** = 160 (suggested for the current continuation)

The complete Bifurcation diagram

The Hopf and the Limit Point bifurcation curves collide in the Bogdanov-Takens point
**AUTO2007 – Some final remarks on the parameter continuation**

- The continuation software AUTO is capable to assess the quantitative and qualitative changes of the asymptotic behavior of time-dependent mathematical models
  - **One parameter continuation**: it allows the detection of coexistence of steady states multiplicity and the occurrence of periodic regimes
  - **Two parameters continuation**: it allows the drawing of bifurcation diagrams, a tool useful for a thorough characterization of the mathematical model under investigation (at least for the regime solutions)

- The dynamical behaviour of the mathematical model can be more complex with respect to the ones here presented (e.g. quasiperiodic and/or chaotic oscillations can occur).

- Even in these cases, AUTO may be helpful to rigorously detect the onset of more complicated dynamical behaviours.

**AUTO2007 as an Optimization Software – Definition of Objective Functions**

- **Example:**
  - Let consider the following objective function, which may be a (reasonable) measure of the reactor performance
    \[
    \phi(\theta) = F \times P \times f(X_{1F})
    \]

- For example, one can consider the following objective function
  \[
  \phi = \frac{x_2}{D\alpha} - 1.0 \cdot x_{1F}^2
  \]

- **Goal**: To find the parameter values \(D\alpha\) (PAR(1)) and \(x_{1F}\) (PAR(4)) leading to the maximum value for the objective function \(\phi\)
AUTO2007 – Definition of Objective Functions

- The parameter-continuation algorithm can be used as an optimization tool by considering one or more parameters as free parameters and the objective function, \( \phi \), as the principal parameter.
- A local extremum of the objective function can be, then, regarded as a limit point.
- As an example, the objective function with respect to \( Da \) is reported in figure
  - The remaining parameters are kept constant
  - A maximum in \( \phi \) is observed when \( Da \sim 1.34 \)

AUTO2007 – How to handle the Objective Functions

- A simple switch of the axis shows that the maximum value of \( \phi \) can be regarded as a singular point:

- indeed the extremum point can be regarded as a limit point (LP) with respect to the additional parameter \( \phi \).
The objective function $\phi$ has to be defined in the subroutine \texttt{FOPT (Function OPTimum)}.

The detection of the extremum of $\phi$ as parameters vary can be established by setting the constant \textbf{IPS $= 5$}.

The detection of the extremum of an objective function depending on $n$ parameters can be regarded with \textsc{AUTO} as a continuation with respect to $(n+1)$ parameters. For the case at hand, a continuation with respect to 3 parameters:

- The objective function $\phi$: principal parameter, it is specified with the parameter \texttt{PAR(10)}
- The Damkohler number \texttt{(PAR(1))}
- The inlet feed biomass concentration $X_{1F}$ \texttt{(PAR(4))}

\textbf{IPS $= 5$}

It defines an optimization problem.

\textbf{Starting from the initial point (IRS $= 0$)}

\textbf{Number of free parameters selected for the current continuation}

\texttt{ICP(1) = 10: the principal parameter for the continuation is the objective function PAR(10).}

In succession the parameters \texttt{PAR(1)} and \texttt{PAR(4)} are considered.
AUTO2007 – Detection of the extremum of the objective function: Results

- First continuation: detection of the Limit Point in the 2D space (FOPT, PAR(1))

- The principal parameter is PAR(10) = FOPT
- A Limit Point is observed when FOPT = 0.47

- The label corresponding to the LP point is #3:
  - The Damkohler (PAR(1)) moves to the initial value towards Da = 1.336
  - Conversely, the X_1F value (PAR(4)) remains constant.

- Second step: continuation of the LP point in the three parameter space (PAR(10), PAR(1), PAR(4)).

AUTO2007 – Detection of the extremum of the objective function: Results

- Schematization of the continuation-optimization procedure

Gray lines represent the objective function with respect to Da for some discrete values of X_1F.
- Red circles are the maxima of the objective function as parameter Da changes.
- The dashed line represents the locus of the maxima (Limit points) traced by the objective function when also the parameter X_1F is varying.
- The Limit Point detected for the dashed line is the maximum value attained by the objective function with a joint variation of the two parameters.
AUTO2007 – Extrema detection: continuation with respect to the second parameter

- Changes to be carried out in the c.bioreatt file in order to run the 2D continuation of the LP point:
  - IRS -> number corresponding to the LP label observed in the previous continuation
  - For the case at hand IRS = 3

- There are no further changes to be accomplished

AUTO2007 – Two parameter continuation for the extremum detection

The pairs (PAR(1), PAR(4)) carried out with the continuation correspond to the dashed curve points previously reported.

It should be noted that both parameters (Da and X1F) are changing along the curve.
AUTO2007 – Final remarks on the optimization

- AUTO2007 allows to:
  - assess the optimal operating parameters for a given generic objective function
  - investigate how the optimal conditions change as other parameters vary

- Drawbacks:
  - There is no warranty that the extremum detected is the absolute maximum
  - The stability of the optimal solution is not checked as in the case of the traditional continuation.

AUTO – Other tools provided by the software

- AUTO can be used to:
  - detect the solutions and investigate the stability of a wide class of parabolic partial differential equations
  - perform the Continuation of global bifurcations (homoclinic bifurcations)
  - perform the optimization of periodic solutions
  - And many other ...
AUTO on the WEB

AUTO is freeware!!

- You can download it on
  - http://indy.cs.concordia.ca/auto/

- A Matlab® version of AUTO has been also recently implemented
  - http://www.mathworks.co.uk/matlabcentral/fileexchange/32210-dynamical-systems-toolbox

Other Continuation Software

- **LOCA**: is (with NOX) a combined package for robustly solving and analyzing large-scale systems of nonlinear equations.

- **MATCONT**: is a tool for Matlab® that continues equilibrium solutions, periodic orbits etc.
  - http://sourceforge.net/projects/matcont

- **XPPAUT**: is a software for the numerical simulation and bifurcation analysis of dynamical systems. Spartan user interface

- **PyDSTool**: is a project that supports symbolic math, optimization, continuation and bifurcation analysis, data analysis, and other tools for modeling
  - http://www2.gsu.edu/~mattrhc/PyDSTool.htm
References
