

An Introduction to



PLAS

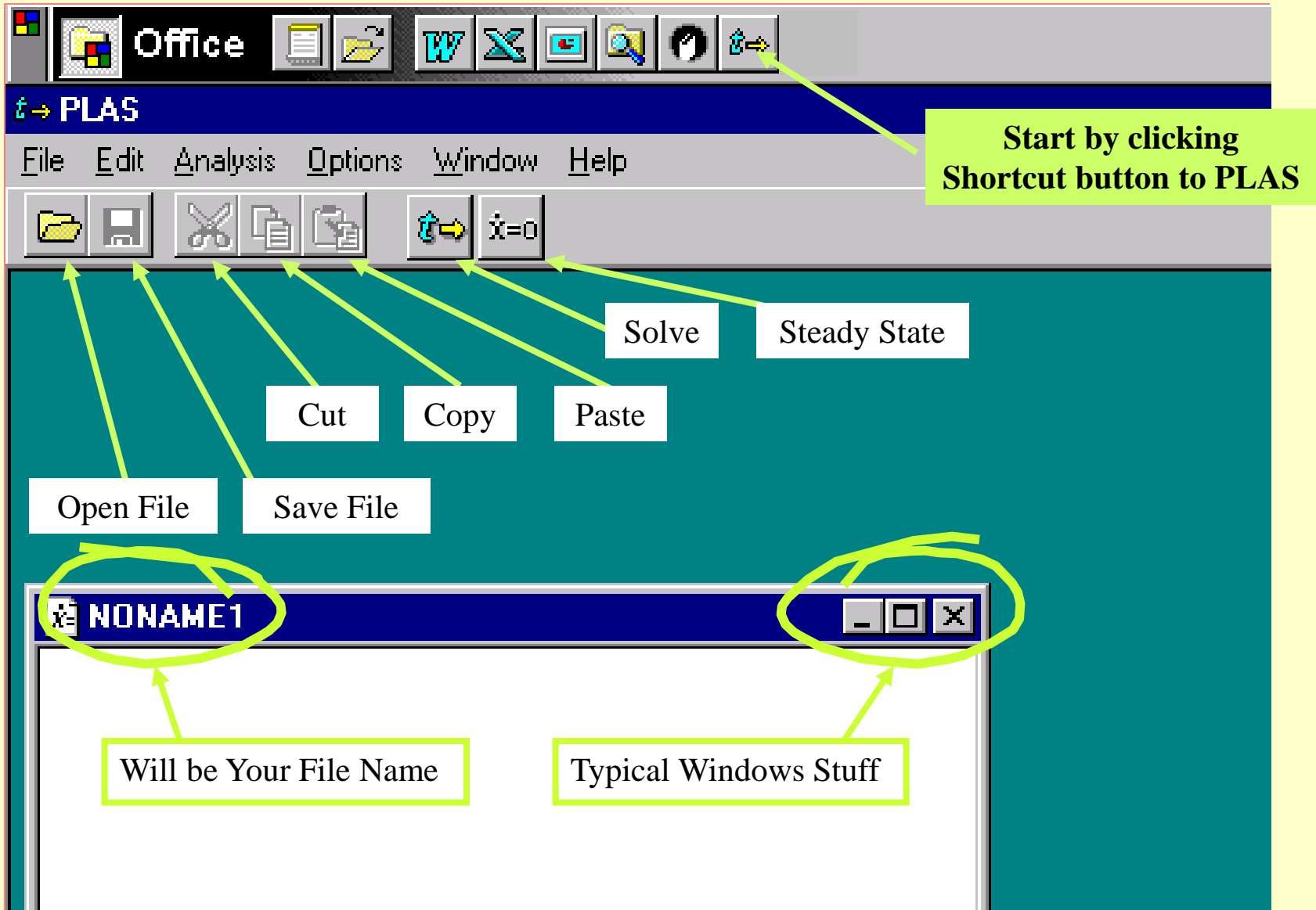
POWER LAW ANALYSIS AND SIMULATION

Copyright: António E.N. Ferreira 2001-2012

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<http://enzymology.fc.ul.pt/software>

Download PLAS and Create Shortcut



Components of a PLAS File

Mandatory

Definition of Differential Equations

Definition of Initial Values

Definition of Parameters

Sometimes Mandatory

Definition of Independent Variables

Optional

Title

Comments

Transformations

“Show only” Option



Template File with Basic Commands (see File AAATemplate)

Start with AAATemplate,
save under another name

```
C:\WINNT\Profiles\voit\Desktop\PLAS 32\PortTemplate.998.ppc
Template // Name: AAATemplate
File Name // Useful as reminder

=====
Definition of differential equations
x' = y - 2 x^p // for p = 0, a power-lawed sine function
y' = 2 x^p - x // for p = 0, a power-lawed cosine function
=====
Initial values, one each
x = 2 // oscillate about 2; sine starts at 2
y = 3 // oscillate about 2; cosine starts at 2 + 1
=====
Definition of parameters
p = .1 // parameter to play with; may be negative
=====
Transformations
z = (1. + ln[x+y])^5/3 + 1 // parameter to play with; may be negative
=====
Solution parameters
t0 = 0 // start point of solution
tf = 50 // end point of solution
hr = .1 // "report interval"
// PLAS computes @ t0, t0+hr, t0+2hr, ... tf
=====
Other commands
!! z
```

Must be the
same names

Statements starting with
// are comments

Arguments of functions
in brackets

“Taboo” names: They
must not be changed

Show z only!

Typical Options

File Edit Analysis Options Window Help

Much is explained here!

Arrangement of Windows

Typical File Options

Typical Edit Options

Steady State Run

Solver Settings

C:\WINNT\Profiles\voit\Desktop\PLAS 32\PortTemplate.998.plc

Template // Name: AAATemplate

Your File Name with Path

File Name // Useful as reminder

=====

A First Dynamic Solution: Click



Progress of solution is shown; often it is too fast to see

The screenshot displays the PLAS software interface. The main window shows a plot of the variable z over time, with the y-axis ranging from 0 to 40 and the x-axis from 0 to 50. The plot shows a damped oscillation starting at approximately 40 and settling around 15. A legend in the top left of the plot area identifies the blue line as z . The status bar at the top of the plot window indicates "100% Done in 47 ms", "Step 69", "Indep. var. 51.29785", "Order 10", and "Step size 1.2999".

The left pane contains the following configuration text:

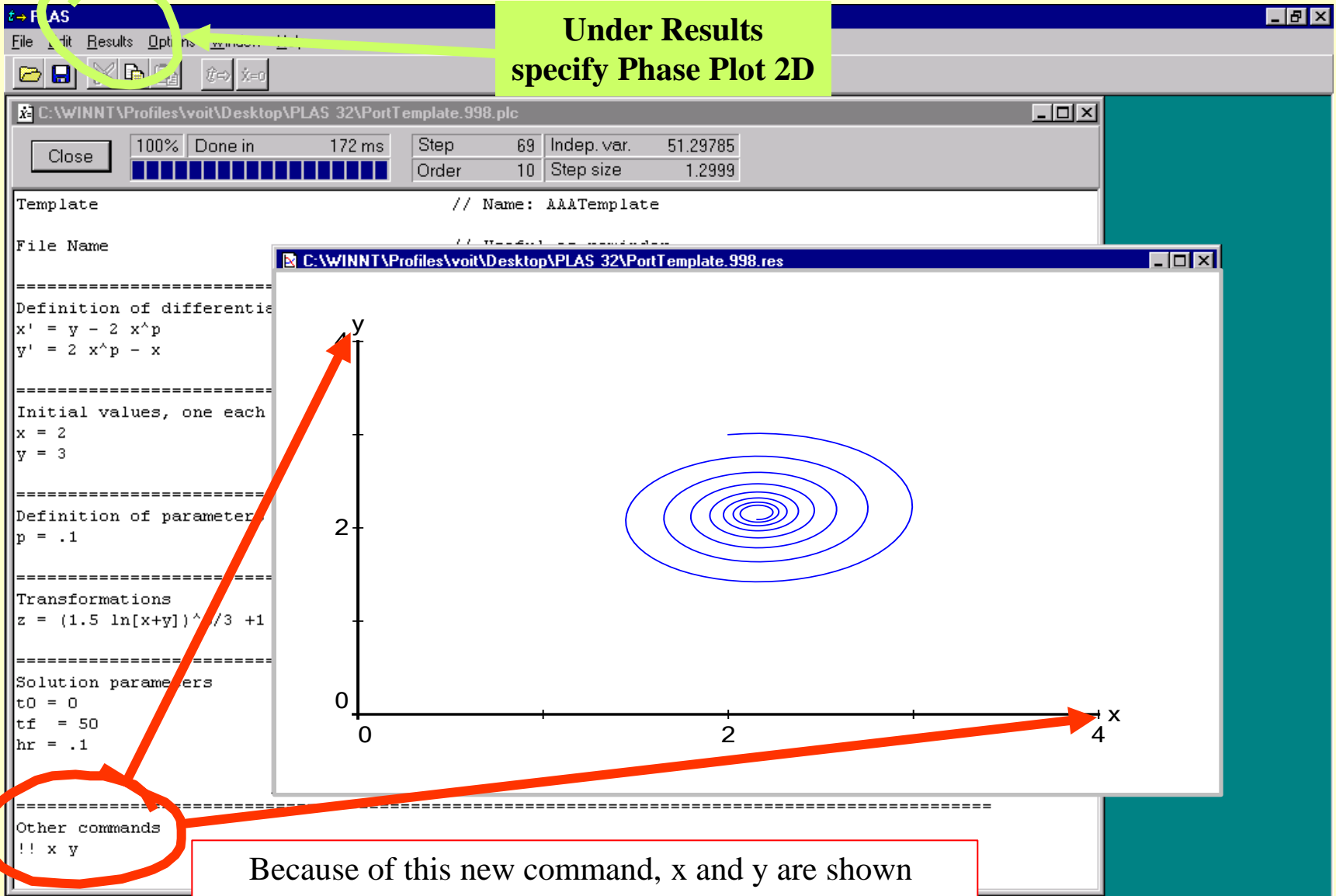
```
Template // Name: AAA_Template
File Name // Name: AAA_Template
-----
Definition of differential equations
x' = y - 2 x^p
y' = 2 x^p - x
-----
Initial values, one each
x = 2
y = 3
-----
Definition of parameter
p = .1
-----
Transformations
z = (1.5 ln[x+y])^5/3 + 1
-----
Solution parameters
t0 = 0
tf = 50
hr = .1
-----
Other commands
!! z
```

Red circles highlight the status bar, the legend entry for z , and the "Other commands" section. A red arrow points from the "Other commands" section to the plot.

Because of this command, only z is shown

Phase Plane Plot

Under Results
specify Phase Plot 2D



Because of this new command, x and y are shown
(need to run the program again, before x and y show up)

Display Options

The screenshot displays the PLAS software interface with three tiled windows. The top window is the menu bar, with the "Window" menu highlighted by a red box and an arrow pointing to a text box labeled "Tiled" windows".

The left window shows a time-series plot of variables x, y, and z over time. The x-axis ranges from 0 to 50, and the y-axis ranges from 0 to 30.2212. The plot shows a large oscillation for z and smaller oscillations for x and y.

The middle window is a command window with the following content:

```
Close 100% Done in 31 ms Ste
Orc

Template
File Name
=====
Definition of differential equations
x' = y - 2 x^p
y' = 2 x^p - x
=====
Initial values, one each
x = 2
y = 3
=====
Definition of parameters
p = .1
=====
Transformations
z = (1.5 ln[x+y])^5/3 +1
=====
Solution parameters
t0 = 0
tf = 50
hr = .1
=====
Other commands
!! x y z
```

The right window shows a phase portrait in the x-y plane. The x-axis ranges from 1.2 to 3, and the y-axis ranges from 1.2 to 3. The plot shows several concentric, roughly elliptical trajectories centered around a point, indicating a limit cycle or a stable point.

Display Options for Comparison

Save each result under a new name; load; tile

Results can be selected and right-click copied

The screenshot displays the PLAS software interface with several windows open:

- Top Left Window:** A time-series plot showing two variables, x and y, over time. The y-axis ranges from 0 to 38.2212, and the x-axis ranges from 0 to 60. Variable x shows a large oscillation, while y shows a much smaller one.
- Top Right Window:** A data table with columns x, y, and z. A green circle highlights the row for time 24.8.
- Bottom Left Window:** A contour plot showing nested loops in a 2D space. A green box with the text "Copied with right-click 'Copy'" is overlaid on the plot.
- Bottom Right Window:** A code editor showing the template for the simulation. The code includes:

```
Template // Name: AAATempla
File Name // Useful as remin
-----
Definition of differential equations
x' = y - 2 x^p // for p = 0, a po
y' = 2 x^p - x // for p = 0, a po
-----
Initial values, one each
x = 2 // oscillate about
y = 3 // oscillate about
-----
Definition of parameters
p = .1 // parameter to pl
```

Internal PLAS Representation; Useful for Debugging

The screenshot shows the PLAS software interface with a 'Steady State' dialog box open. The main window displays the following code:

```
Template
// Name: AAATemplate
File Name
// User: ...
=====
Definition of differential
x' = y - 2 x^p
y' = 2 x^p - x
=====
Initial values, one each
x = 2
y = 3
=====
Definition of parameters
p = .1
=====
Transformations
z = (1.5 ln[x+y])^5/3 + 1
=====
Solution parameters
t0 = 0
tf = 50
hr = .1
=====
Other commands
!! x y z
```

The 'Steady State' dialog box has the following content:

System is a full S-system.

General information | Steady State | Variables sensitivity | Fluxes sensitivity

NAMES		
Name	value	internal
x	2	X1
y	3	X2
z	28.33418805	transf 1
p	0.1	const 3
t0	0	const 5
hr	0.1	const 7
tf	50	const 10

INTERNAL REPRESENTATION

```
X1' = X2 - 2 (X1^0.1)
X2' = 2 (X1^0.1) - X1
```

Annotations: A green circle highlights the 'X=0' button in the toolbar. A red circle highlights the differential equations in the main window. Another red circle highlights the 'INTERNAL REPRESENTATION' section in the dialog box. A large red arrow points from the differential equations to the internal representation, with the word 'Compare!' written in large red text above it.

Display of Steady-State Features ($\dot{x}=0$)

The screenshot shows the PLAS software interface with a 'Steady State' dialog box open. The dialog box contains the following information:

System is a full S-system.

General information | Steady State | Variables sensitivities | Fluxes sensitivities

Variable	St	Flux	E-value
x	2.160119	2.160119	1
y	2.160119	2.160119	1

Eigenvalues:

Re	Im
-0.05	0.9473648
-0.05	-0.9473648

Annotations:

- A red box highlights the $\dot{x}=0$ button in the top toolbar.
- A yellow box with the text "Select and right-click to copy" points to the Steady State dialog box.
- A blue box with the text "z not listed, since it is a transformation" points to the transformation equation $z = 1.5 \ln(x+y)^{5/3}$ in the background window.
- A brown box with the text "Stable" points to the real part of the eigenvalues (-0.05).
- A teal box with the text "Oscillations" points to the imaginary part of the eigenvalues (0.9473648).

Background window content:

```
PLAS
File Edit Analysis Options Window Help
C:\WINNT\Profiles\voit... 32\PortTemplate.998.plc
Template
File Name
Name: AAATemplate
Definition of differential equations
x' = y - 2 x^p
y' = 2 x^p - x
Initial values, one for each variable
x = 2
y = 3
Definition of parameters
p = .1
Transformations
z = 1.5 ln(x+y)^5/3
Solution parameters
t0 = 0
tf = 50
hr = .1
Other commands
!! x y z
```

Display of Variable Sensitivities

PLAS

File Edit Analysis Options Window Help

$\dot{x}=0$

C:\WINNT\Profiles\...

Template

File Name

Definition of u

$x' = y - 2x^p$
 $y' = 2x^p - x$

Initial values,
 $x = 2$
 $y = 3$

Definition of p
 $p = .1$

Transformations
 $z = (1.5 \ln[x+y$

Solution paramete
 $t_0 = 0$
 $t_f = 50$
 $h_r = .1$

Steady State

System is a full S-system.

Hide if absolute value < 0.01

General information | Steady State | Variables sensitivities | Fluxes sensitivities

	x	y
alpha(1)	---	-1.00000
beta(1)	---	1.00000
alpha(2)	1.11111	0.11111
beta(2)	-1.11111	-0.11111
g(1,2)	---	-0.77016
h(1,1)	---	0.07702
g(2,1)	0.08557	---
h(2,1)	-0.85574	-0.08557

OK

// PLAS computes @ t0, t0+hr, t0+2hr, ... tf

Hide insignificant quantities

Select and right-click to copy

Comparative Simulation Studies

Template

File Name

=====
Definition of differential equations
 $x' = y - 2x^p$
 $y' = 2x^p - x$
=====
Initial conditions
 $x = 2$
=====
Definition of parameters
 $p = .01$
=====
Transformations
 $\ln(x+y)^5$
=====
Solution parameters
 $t0 = 0$
 $tf = 50$
 $hr = .1$
=====
Other commands

C:\WINNT\Profiles\voit\Desktop\PLAS 32\PortTemplate.998.res

Save under a new name

Study role of parameter p

z

40

20

0

0 25 50

Comparative Simulation Studies (Cont'd)

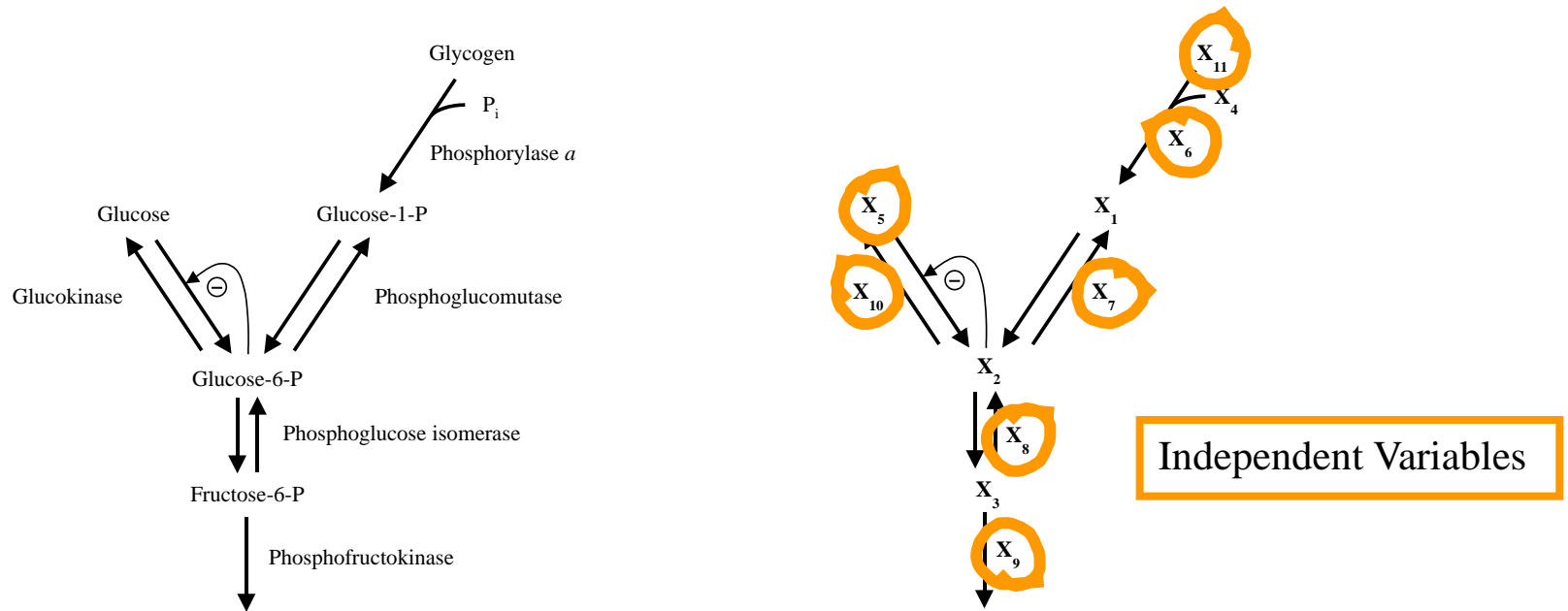
The screenshot displays the PLAS software interface. The main window shows a graph of two oscillating variables, z (red line) and $1:z$ (blue line), over time from 0 to 50. The y-axis ranges from 0 to 40. The graph shows two oscillating curves. The blue curve, labeled $1:z$, has a higher frequency and amplitude, with a peak value of approximately 38. The red curve, labeled z , has a lower frequency and amplitude, with a peak value of approximately 20. The parameter p is set to 0.01 for the blue curve and 0.1 for the red curve. The graph is titled "C:\WINNT\Profiles\voit\Desktop\PLAS 32\PortTemp13.998.res".

The command window on the left contains the following code:

```
Template  
File Name  
-----  
Definition of differ  
x' = y - 2 x^p  
y' = 2 x^p - x  
-----  
Initial values, one e  
x = 2  
y = 3  
-----  
Definition of paramet  
p = .01  
-----  
Transformations  
z = (1.5 ln[x+y])^5/3  
-----  
Solution parameters  
t0 = 0  
tf = 50  
hr = .1  
-----  
Other commands
```

A yellow callout box points to the 'Merge from file' icon in the PLAS toolbar, with the text: "Specify 'Merge from file' to import saved graph".

Example: Initial Steps of Glycolysis and Glycogenolysis*



GMA Model

$$\begin{aligned} \dot{X}_1 &= 0.077884314 X_4^{0.66} X_6 - 1.062708258 X_1^{1.53} X_2^{-0.59} X_7 \\ \dot{X}_2 &= 0.585012402 X_1^{0.95} X_2^{-0.41} X_5^{0.32} X_7^{0.62} X_{10}^{0.38} \\ &\quad - 7.93456 \times 10^{-4} X_2^{3.97} X_3^{-3.06} X_8 \\ \dot{X}_3 &= 7.93456 \times 10^{-4} X_2^{3.97} X_3^{-3.06} X_8 - 1.05880847 X_3^{0.3} X_9 \end{aligned}$$

* Cascante and Torres (unpublished); see details and references in:
 Voit, E.O.: *Computational Analysis of Biochemical Systems*, Cambridge University Press, 2000.

PLAS File for Example

A Model of the First Steps of Glycolysis (Casacante and Torres)

```
X1' = .077884314 X4^0.66 X6 - 1.062708258 X1^1.53 X2^(-0.59) X7  
X2' = .035012402 X1^0.95 X2^-0.41 X5^0.32 X7^0.62 X10^0.38 - >>  
> p X2^3.97 X3^(-3.06) X8  
X3' = p X2^3.97 X3^(-3.06) X8 - 1.05880847 X3^0.3 X9
```

```
X1 = .067  
X2 = .465  
X3 = .15  
X4= 10  
X5= 5  
X6= 3  
X7= 40  
X8= 136  
X9= 2.86  
X10 = 4
```

```
p= .000793456
```

```
&& X4 X5 X6 X7 X8 X9 X10
```

```
V1 = 1.05880847 X3^0.3 X9  
V5 = .038706421 X2^(-0.1) X5^.84 X10  
V7 = .077884314 X4^0.66 X6
```

```
t0 = 0  
tf = .1  
hr = 0.1
```

```
!! x y z
```

Continuation Symbol

Use Symbol
Instead of Number

Independent variables;
made explicit for
log gain computation

Define to report dynamics
of these fluxes

Sensitivity Analysis for Example

C:\PLAS '98\GlycolN2.plc

Glycolysis Model

$$X1' = .077884314 X4^{0.66} X6 - 1.062708258 X1^{1.53} X2^{(-0.59)} X7$$
$$X2' = .585012402 X1^{0.95} X2^{-0.41} X5^{0.32} X7^{0.62} X10^{0.38} >>$$
$$>> - p X2^{3.97} X3^{(-3.06)} X8$$
$$X3' = p X2^{3.97} X3^{(-3.06)} X8 - 1.05880847 X3^{0.3} X9$$

X1 = .067
X2 = .165
X3 = .15
X4 = 10
X5 = 5
X6 = 3
X7 = 40
X8 = 136
X9 = 2.86
X10 = 4

p = .000793456

&& X4 X5 X6 X7 X8 X9 X10

$$V1 = 1.05880847 X3^{0.3} X9$$
$$V5 = .038706421 X2^{(-0.1)} X5^{.84} X10$$
$$V7 = .077884314 X4^{0.66} X6$$

t0 = 0
tf = .1
hr = 0.1

!! x y z

Steady State

System is a full S-system.

Hide if absolute value < 0.01

General information Steady State Variables sensitivities Fluxes sensitivities

	X1	X2	X3
X4	0.82831	1.02334	1.21621
X5	0.30995	0.80377	0.94969
X6	1.25501	1.55960	1.84274
X7	-0.65448	---	---
X8	-0.08648	-0.22427	0.03264
X9	-0.88211	-2.28751	-3.00042
X10	0.36807	0.95448	1.12776
alpha(1)	1.25501	1.55960	1.84274
beta(1)	-1.25501	-1.55960	-1.84274
alpha(2)	0.96859	2.51178	2.96778
beta(2)	-0.96859	-2.51178	-2.96778

OK

Representation of Sensitivities in Excel and PowerPoint

Pick up Data
from PLAS



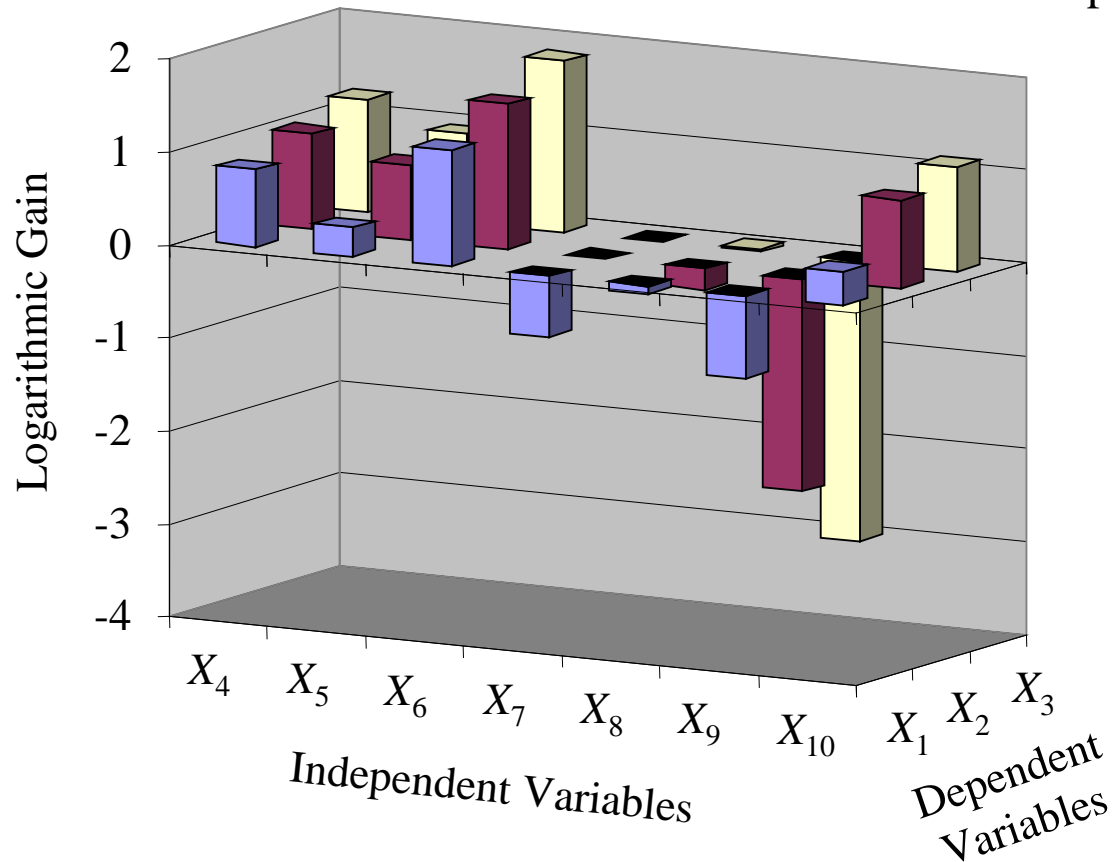
Import into Excel



Create 3D Bar Graph



Import into PowerPoint



Dynamics: Blue Sky Catastrophe (see Chapter 2)

```
C:\WINNT\Profiles\voit\Desktop\PLAS 32\BlueSky.plc
Blue Sky Catastrophe // x'' + 0.25 x' - x^3 = A sin t
File BlueSky1.plc

x' = y // y equals x-dot: one 2nd order >> two 1st order
y' = A (s-2) - 0.25 y + x - x^3
s' = c - 2 // power-lawed sine function
c' = 2 - s // power-lawed cosine function

x = .0101 // guess this to get started
y = .01 // guess this to get started
s = 2 // sine, starting @ 0
c = 3 // corresponding cosine, starting @ 1
A = 0.265 //##### This is the one ##### // parameter to play with //

t0 = 0
tf = 2000 // guess this to get started
hr = .1
```

Use of LSODA Solver for Stiff or Non-Power-Law Systems

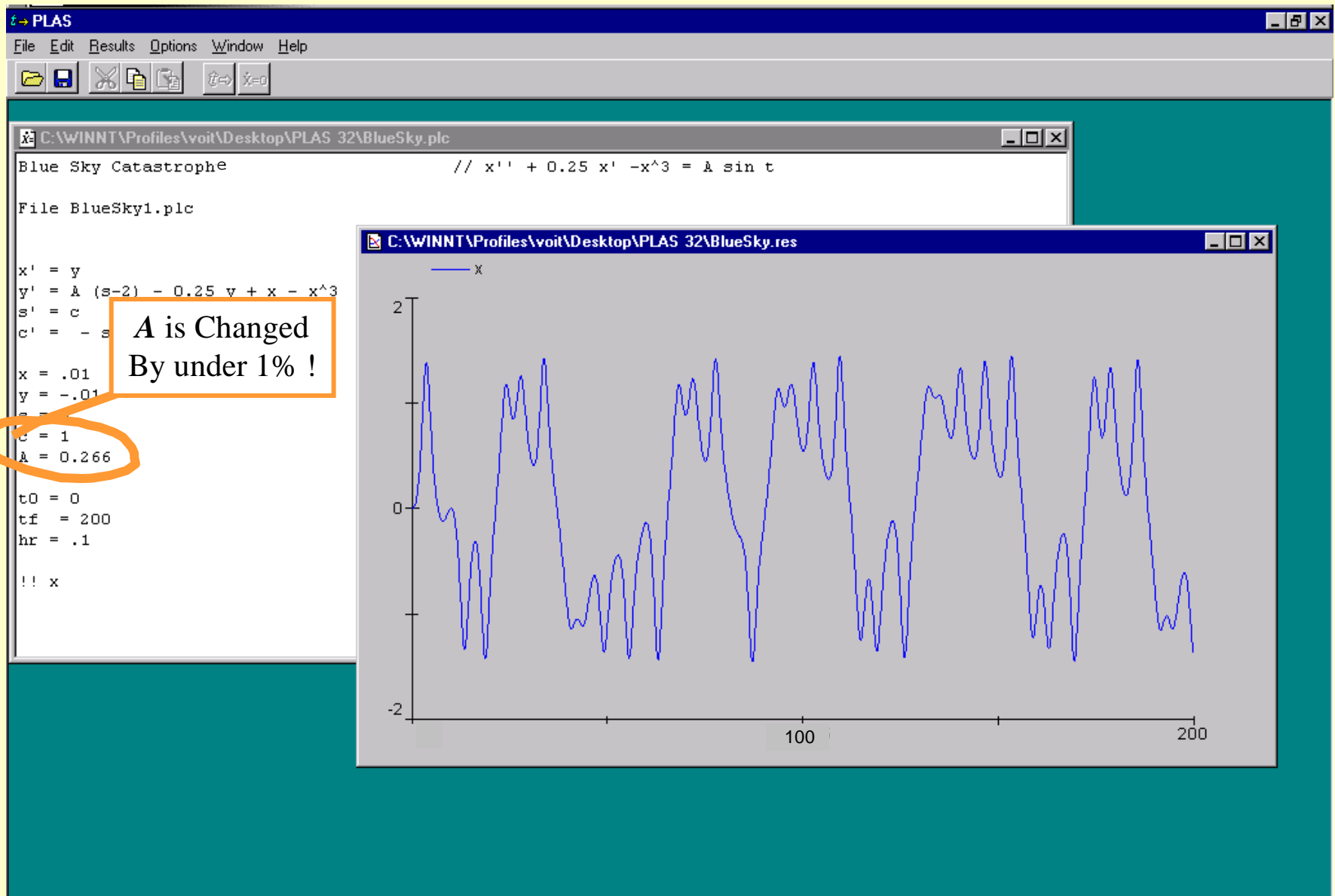
Switch to LSODA Method

The screenshot displays the PLAS software interface. The main window shows a code editor with the following content:

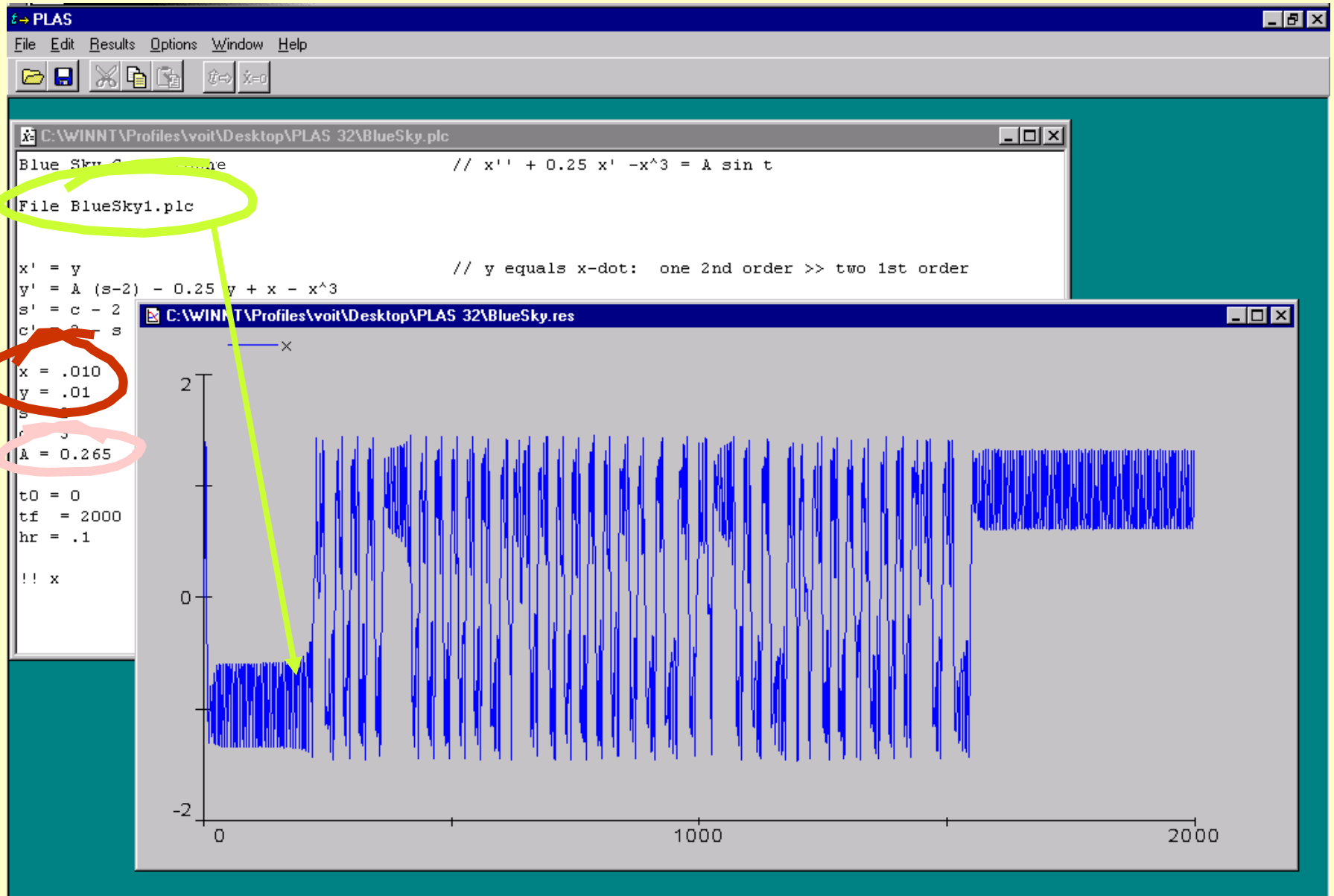
```
Blue Sky Catastrophe // x'' + 0.25 x' - x^3 = A sin t
File BlueSky1.plc
x' = y
y' = A (s-2) - 0.25 y + x - x^3
s' = c
c' = -s
x = .01
y = .01
s = 0
c = 1
A = 0.264
t0 = 0
tf = 200
hr = .1
!! x
```

A yellow circle highlights the 'Results' menu item in the top toolbar, with an arrow pointing to the text 'Switch to LSODA Method'. An orange box highlights the line 'A = 0.264' in the code, with a text box containing 'Test responses to changes in A; start with 0.264'. A red box highlights the plot window, which shows a blue line representing the variable 'x' over time. The plot shows a series of oscillations that start with a large initial transient and then settle into a steady, stable oscillation. A text box in the plot area says 'Nice, stable oscillations!'.

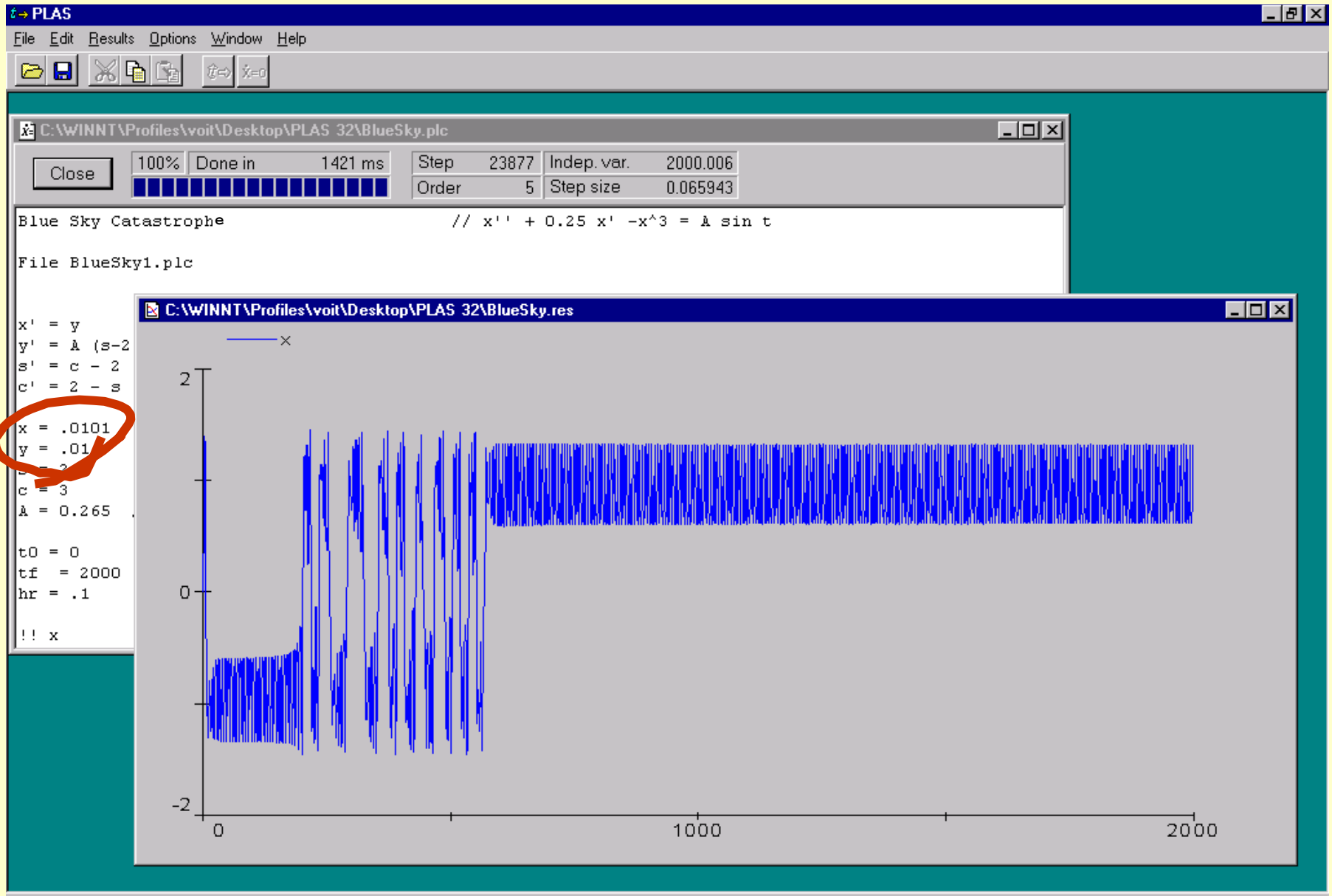
Dynamics is Extremely Sensitive to Changes in Parameter A



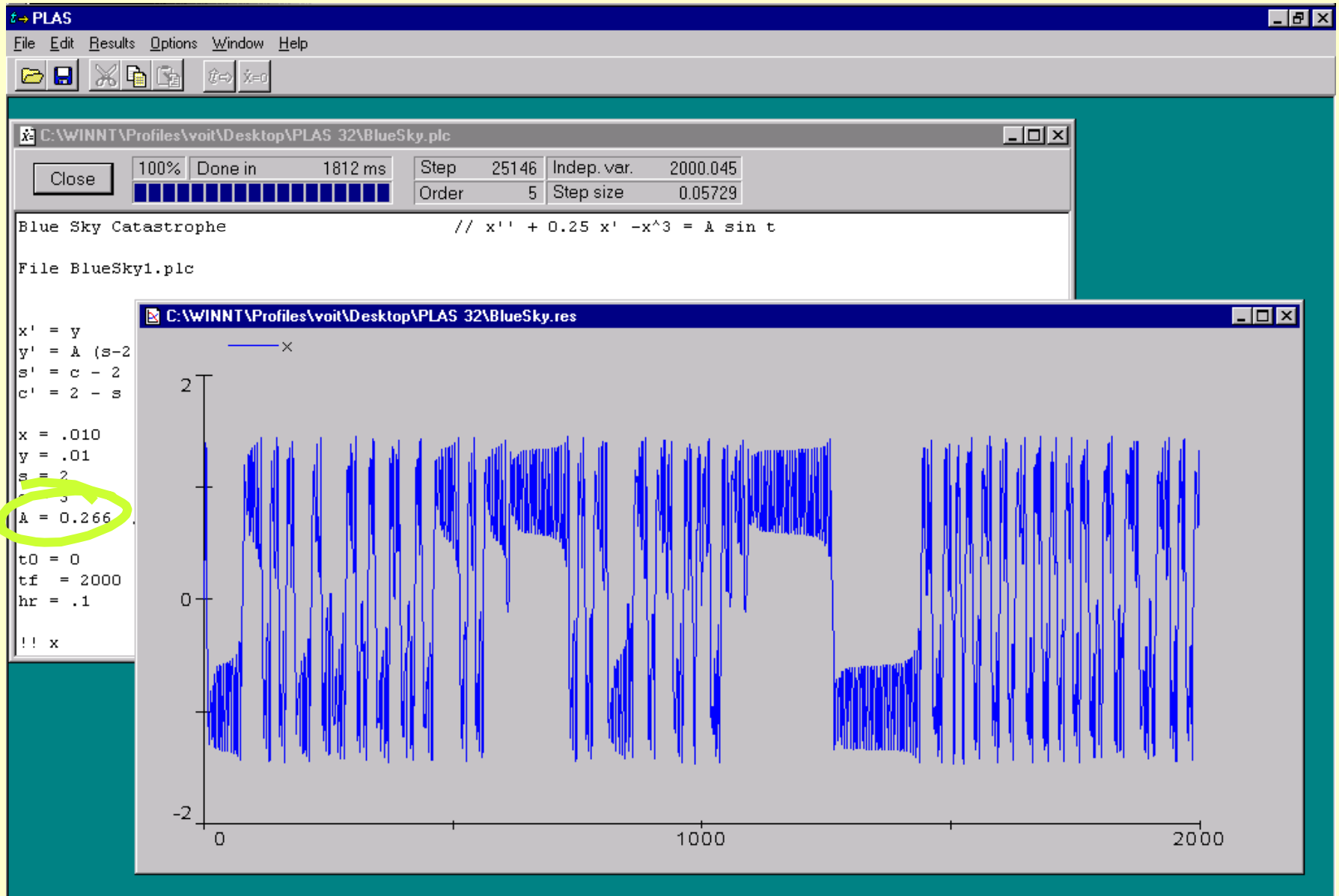
Dynamics is Extremely Sensitive to Changes in Initial Values



Dynamics is Extremely Sensitive to Changes in Initial Values (Cont'd)

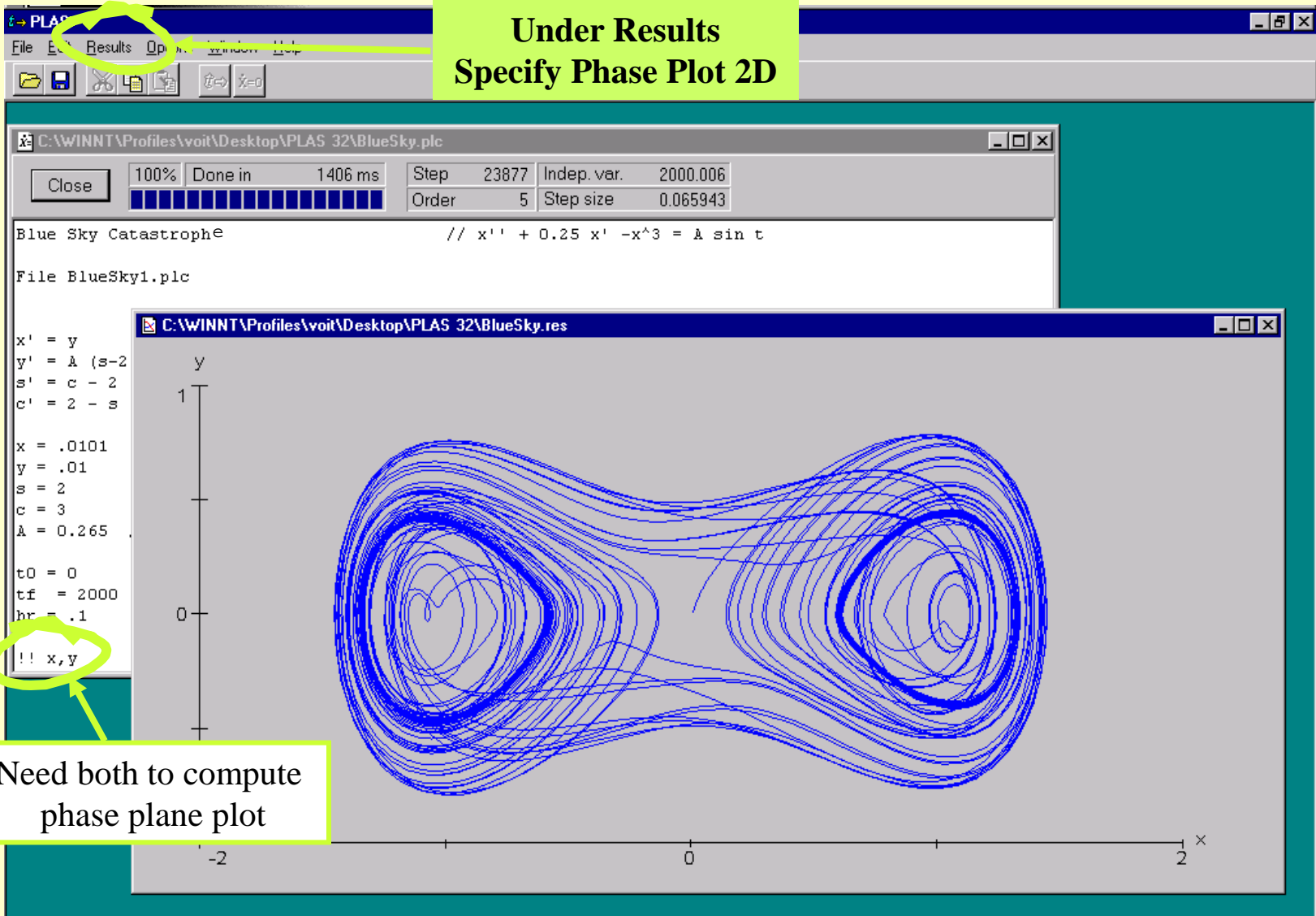


Chaotic Dynamics is Extremely Sensitive (cont'd)



Phase-Plane Plot of Chaotic System

Under Results
Specify Phase Plot 2D



Pseudo-3D Plot of the Chaotic System

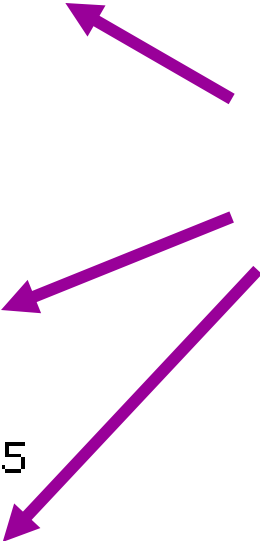
```
x' = y  
y' = λ (s-2) - 0.25 y + x - x^3  
s' = c - 2  
c' = 2 - s  
t' = 0.002
```

```
x = .010  
y = .01  
s = 2  
c = 3  
t = 0.0
```

```
λ = 0.265
```

```
!! x y t
```

Create explicit variable for time
(scaled)



Pseudo-3D Plot of the Chaotic System

