An Introduction to

PLAS

POWER LAW ANALYSIS AND SIMULATION

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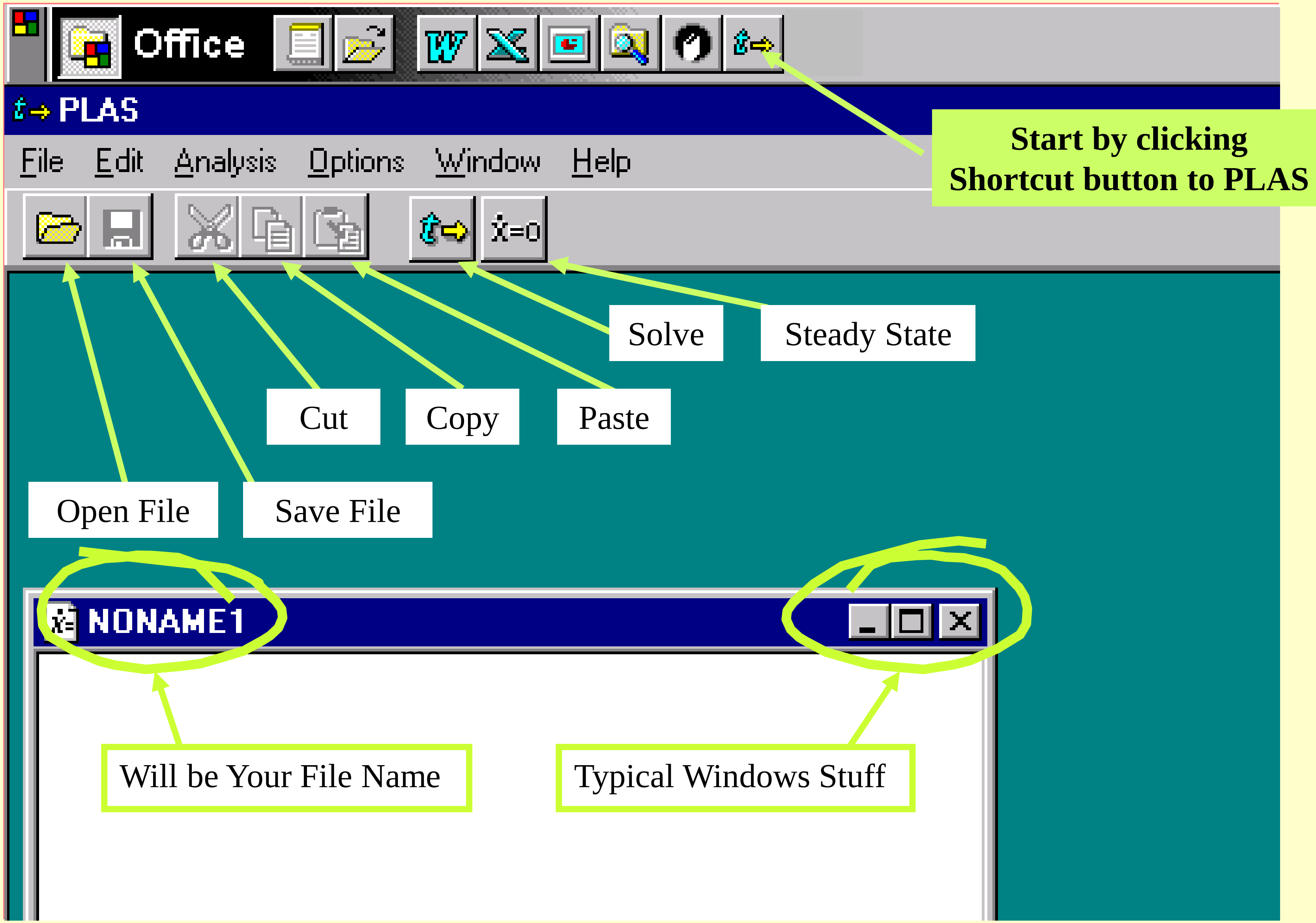
Download PLAS and Create Shortcut



Components of a PLAS File

Mandatory

Definition of Differential Equations

Definition of Initial Values

Definition of Parameters

Sometimes Mandatory

Definition of Independent Variables

Optional

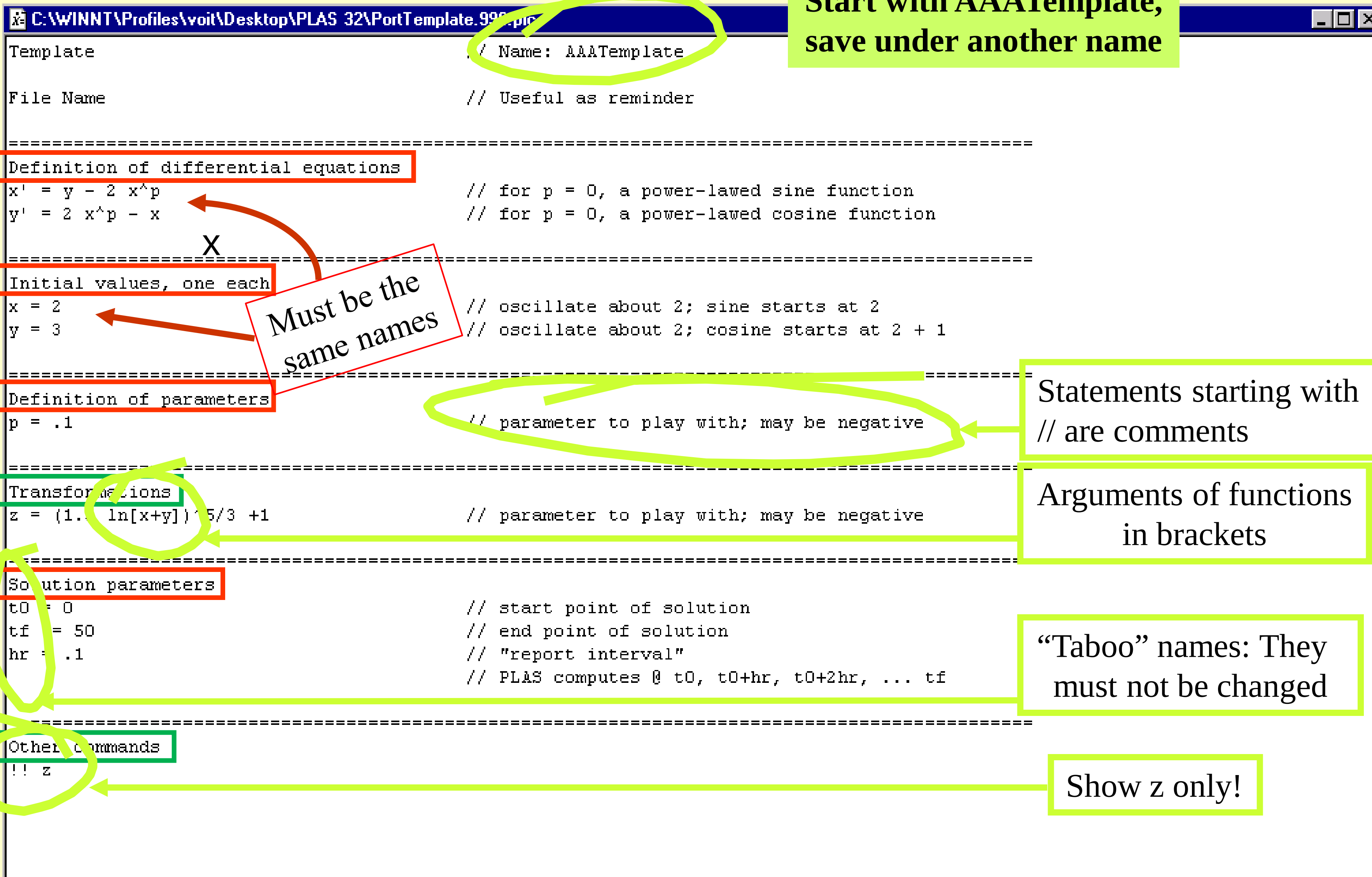
Title

Comments

Transformations

“Show only” Option

Template File with Basic Commands (see File AAATemplate)



```
C:\WINNT\Profiles\voit\Desktop\PLAS 32\PortTemplate.99

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
```


Start with AAATemplate, save under another name

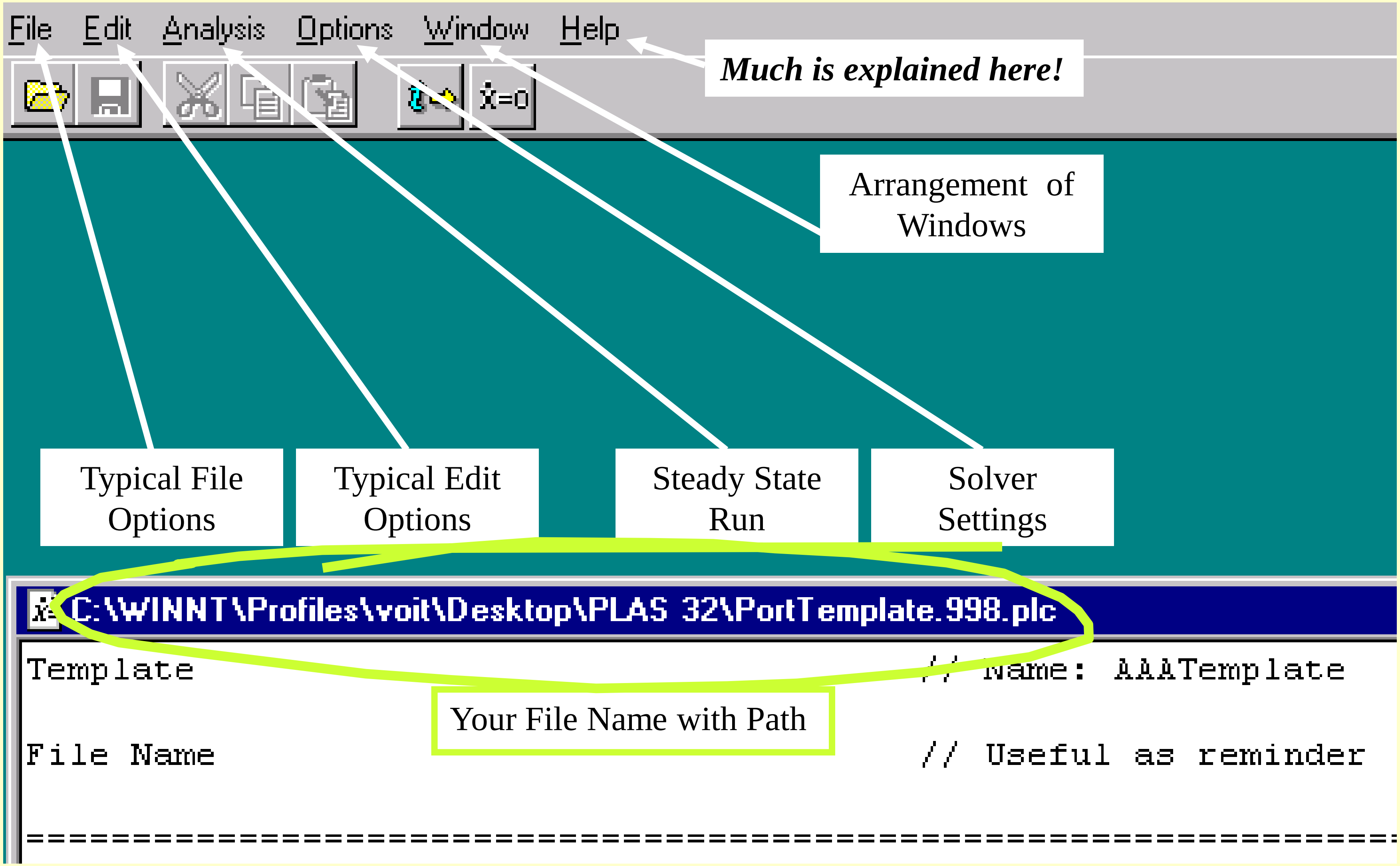
Statements starting with // are comments

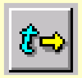
Arguments of functions in brackets

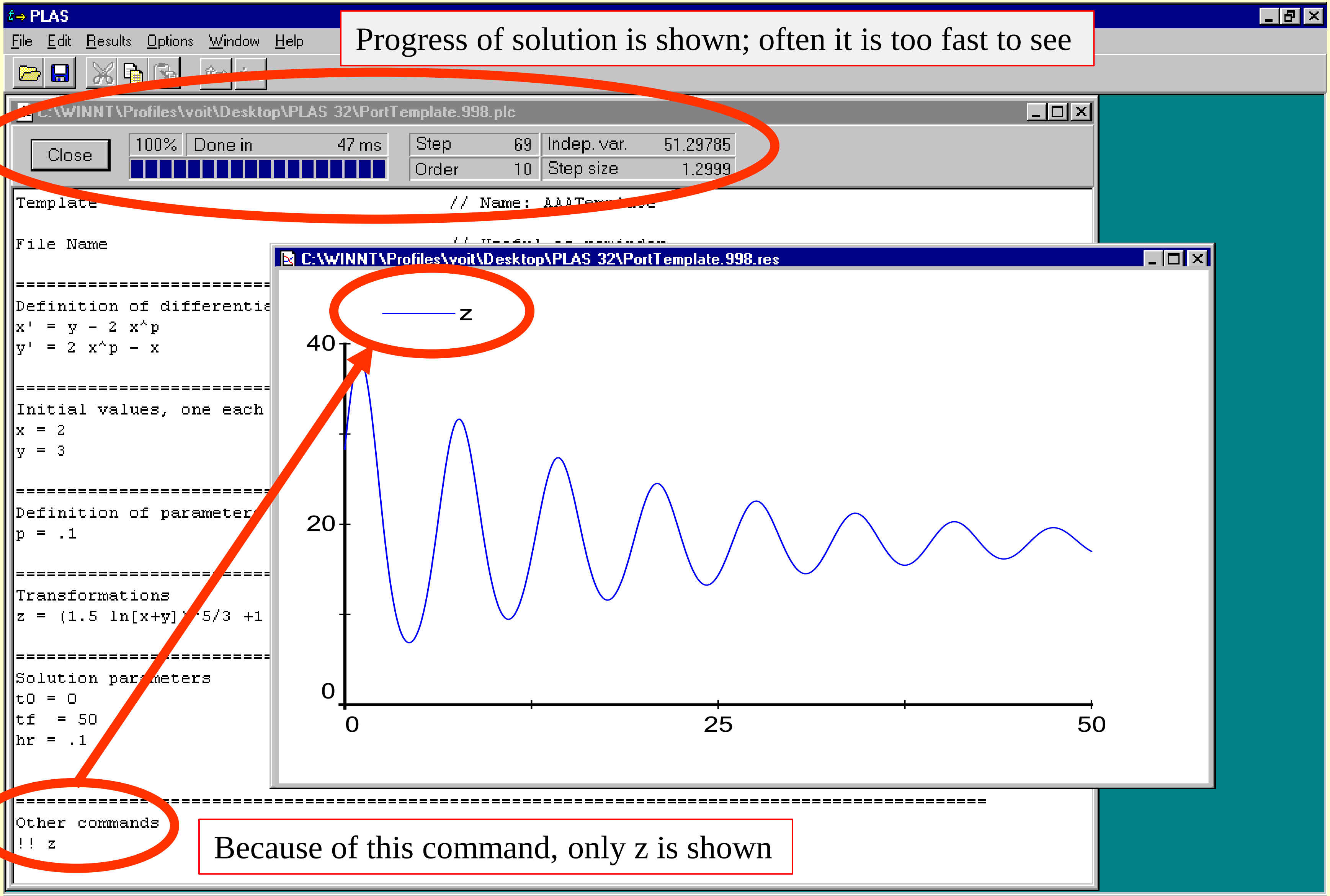
“Taboo” names: They must not be changed

Show z only!

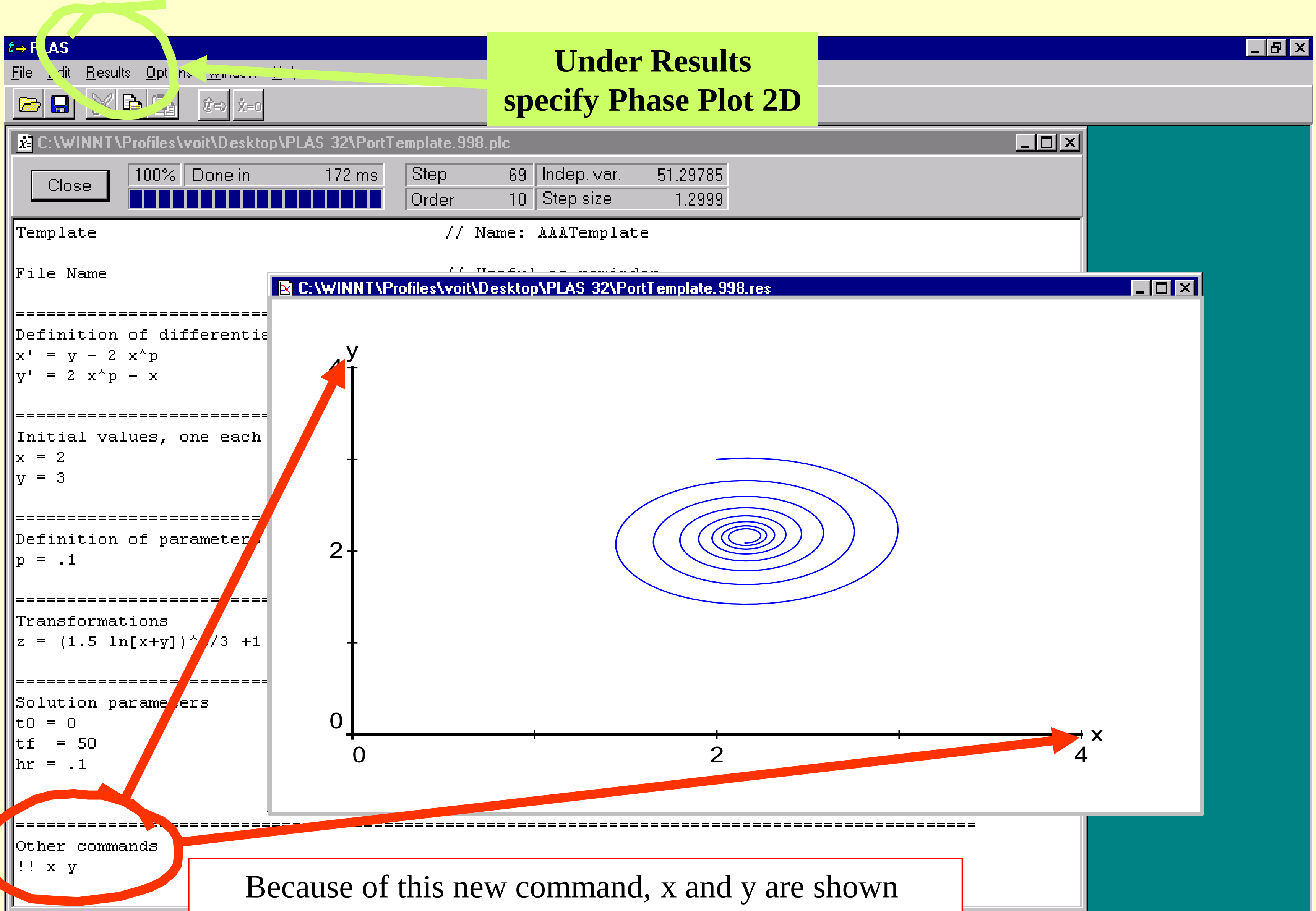
Typical Options



A First Dynamic Solution: Click 



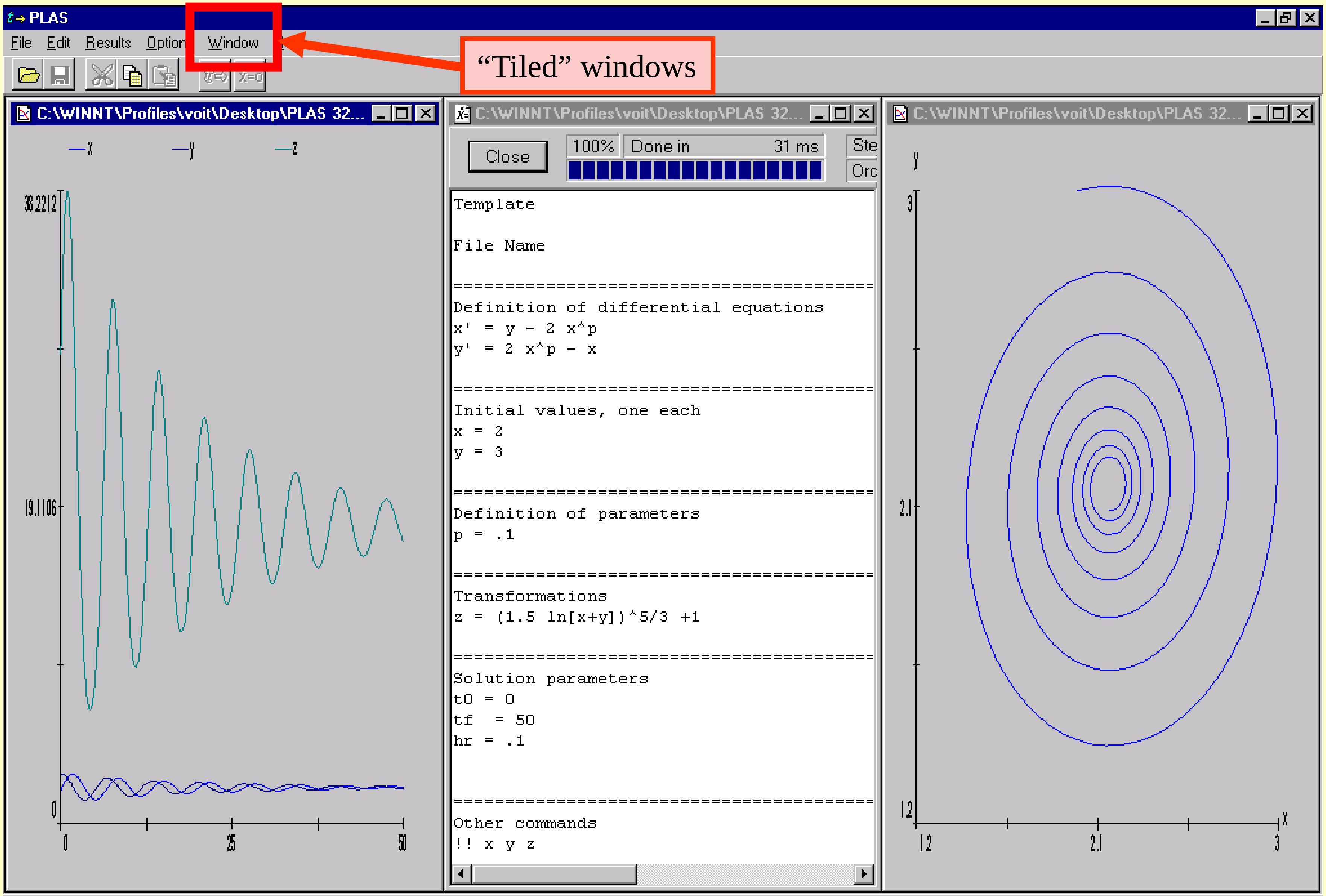
Phase Plane Plot



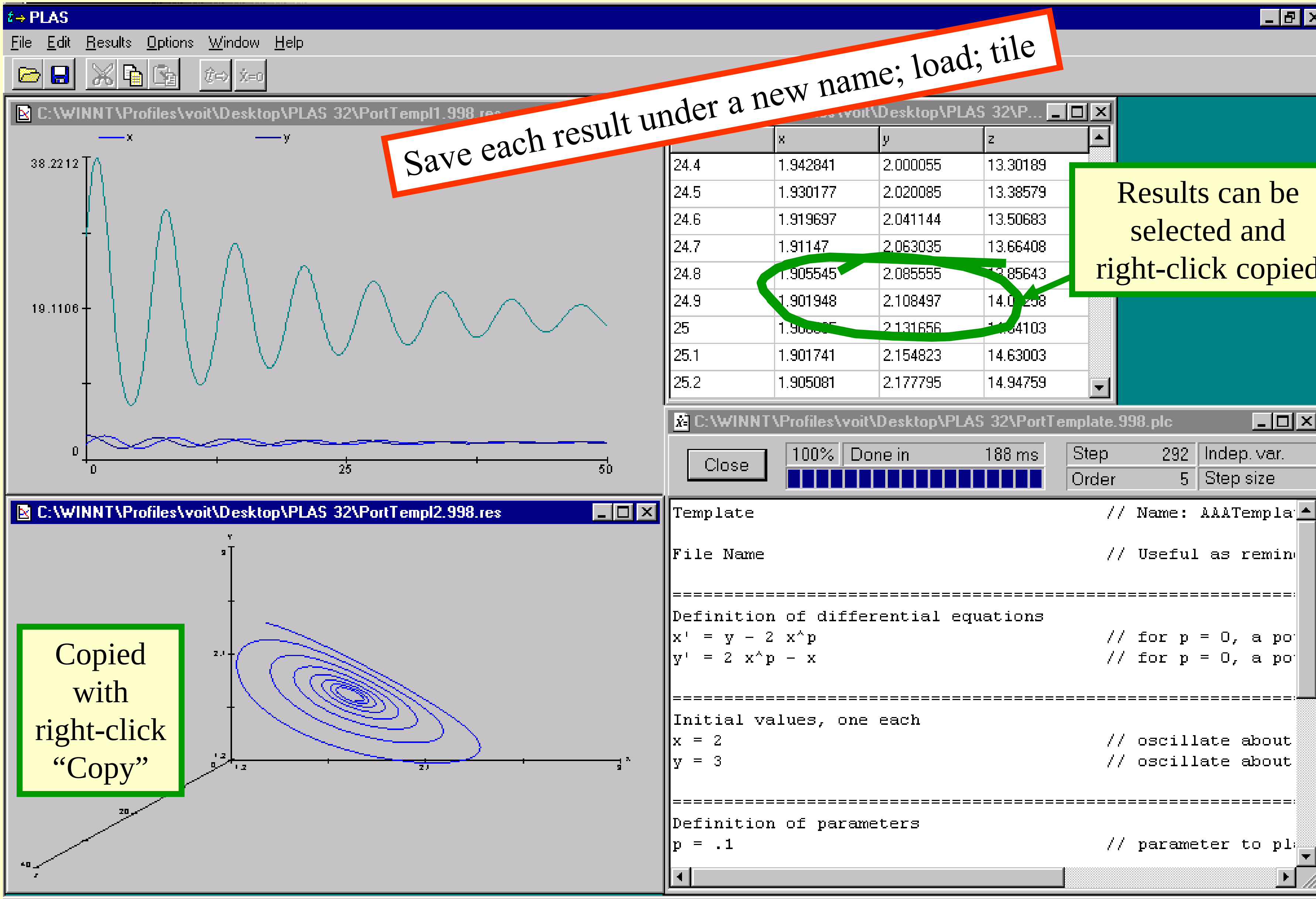
Under Results specify Phase Plot 2D

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

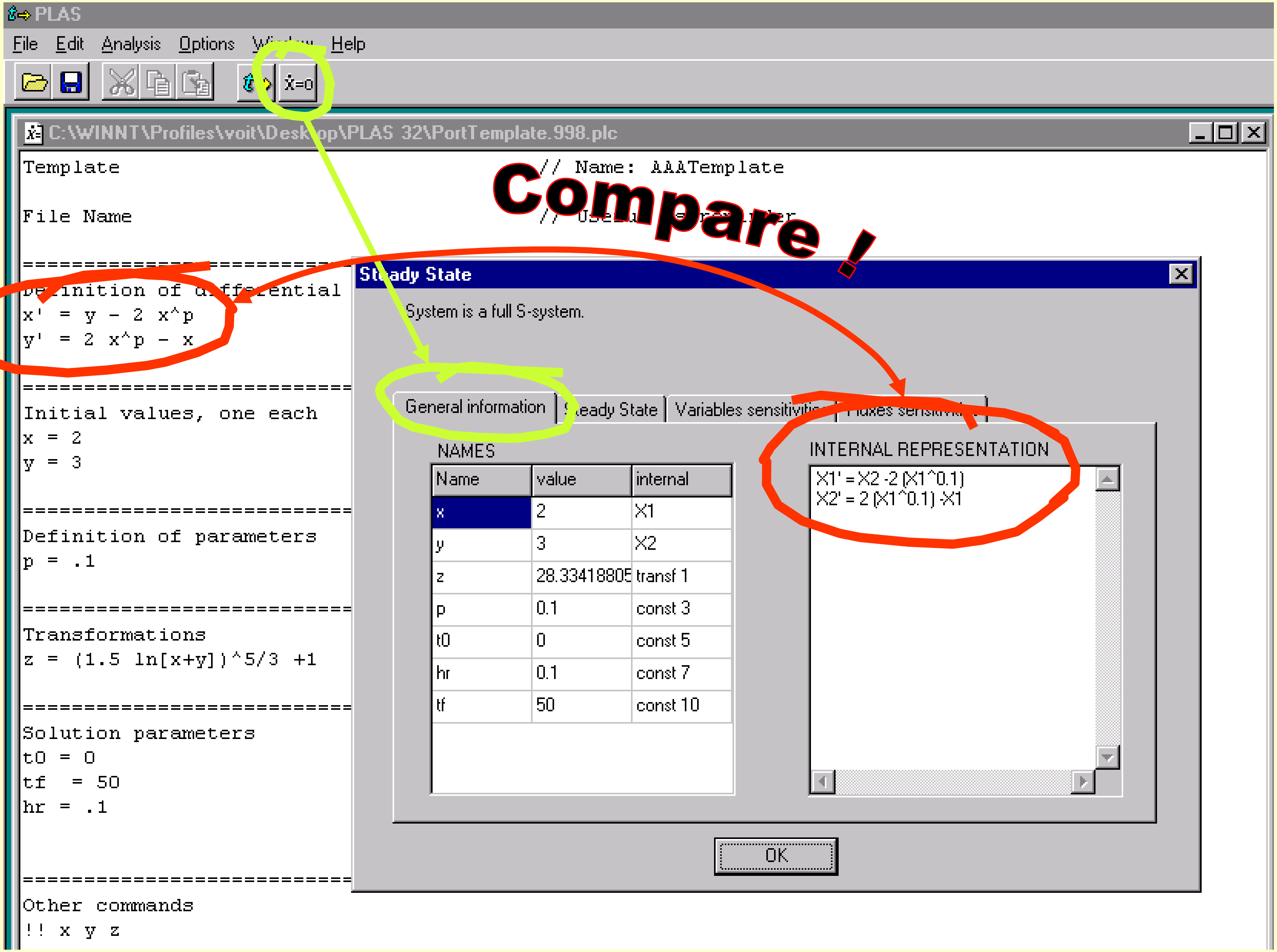
Display Options



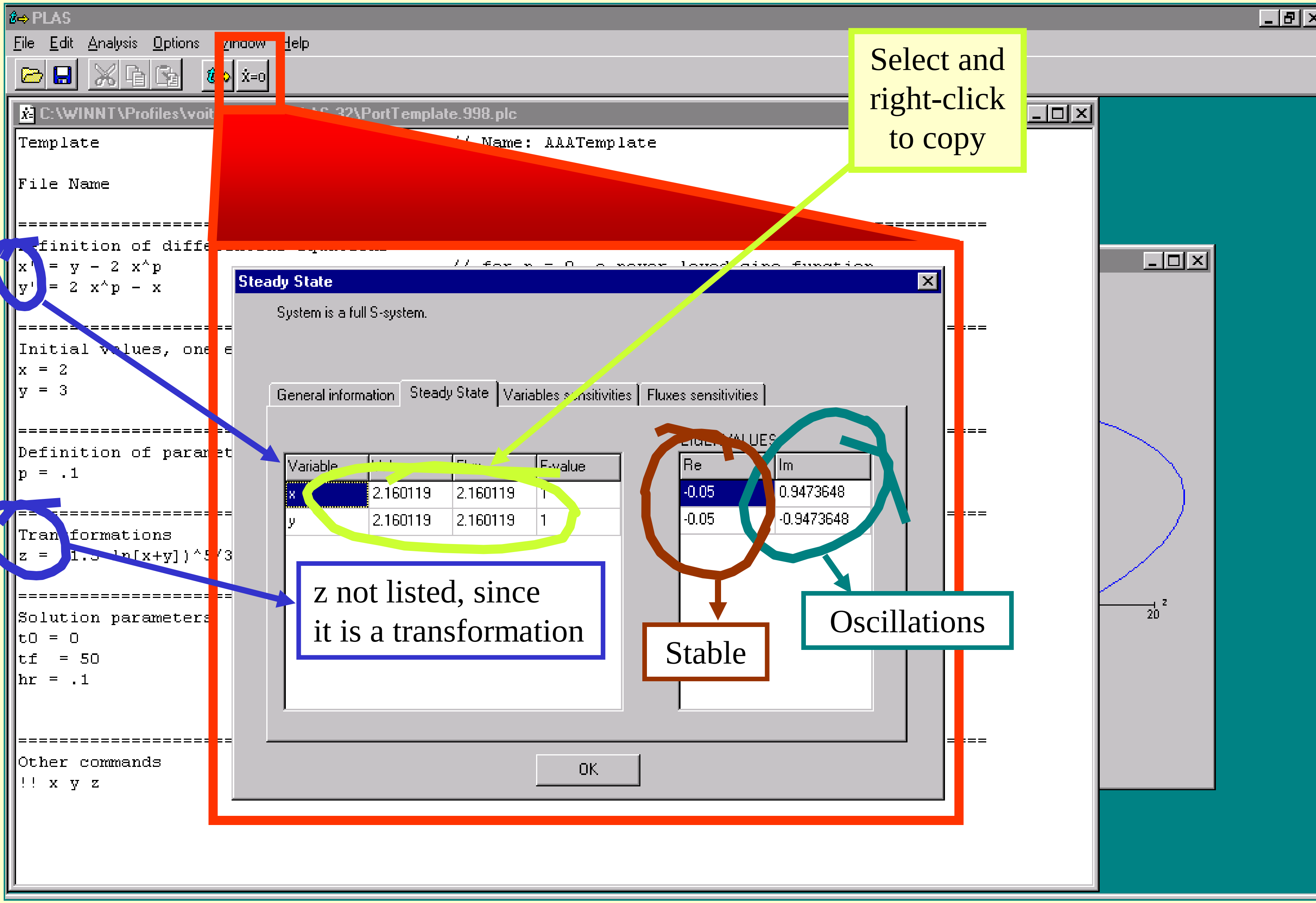
Display Options for Comparison



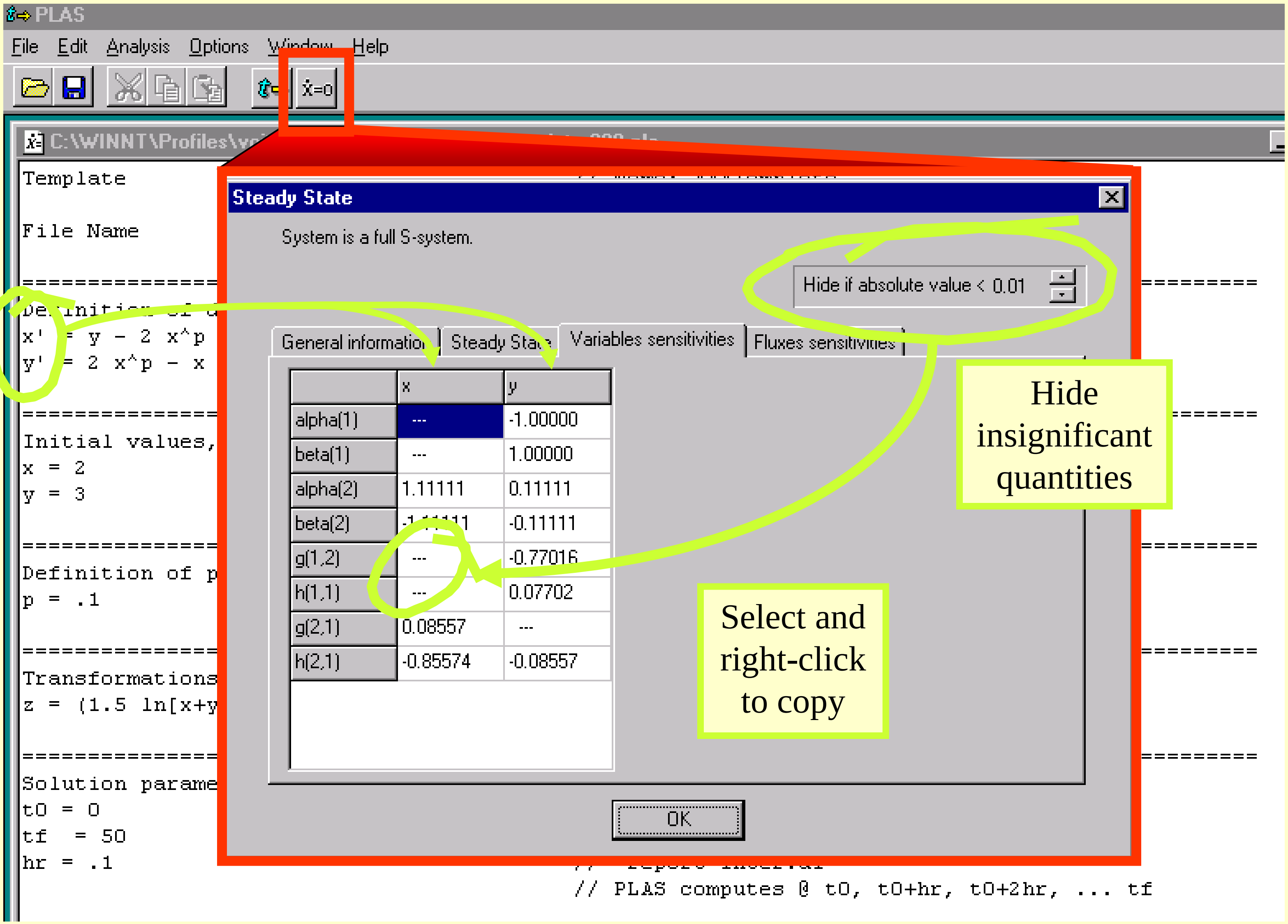
Internal PLAS Representation; Useful for Debugging



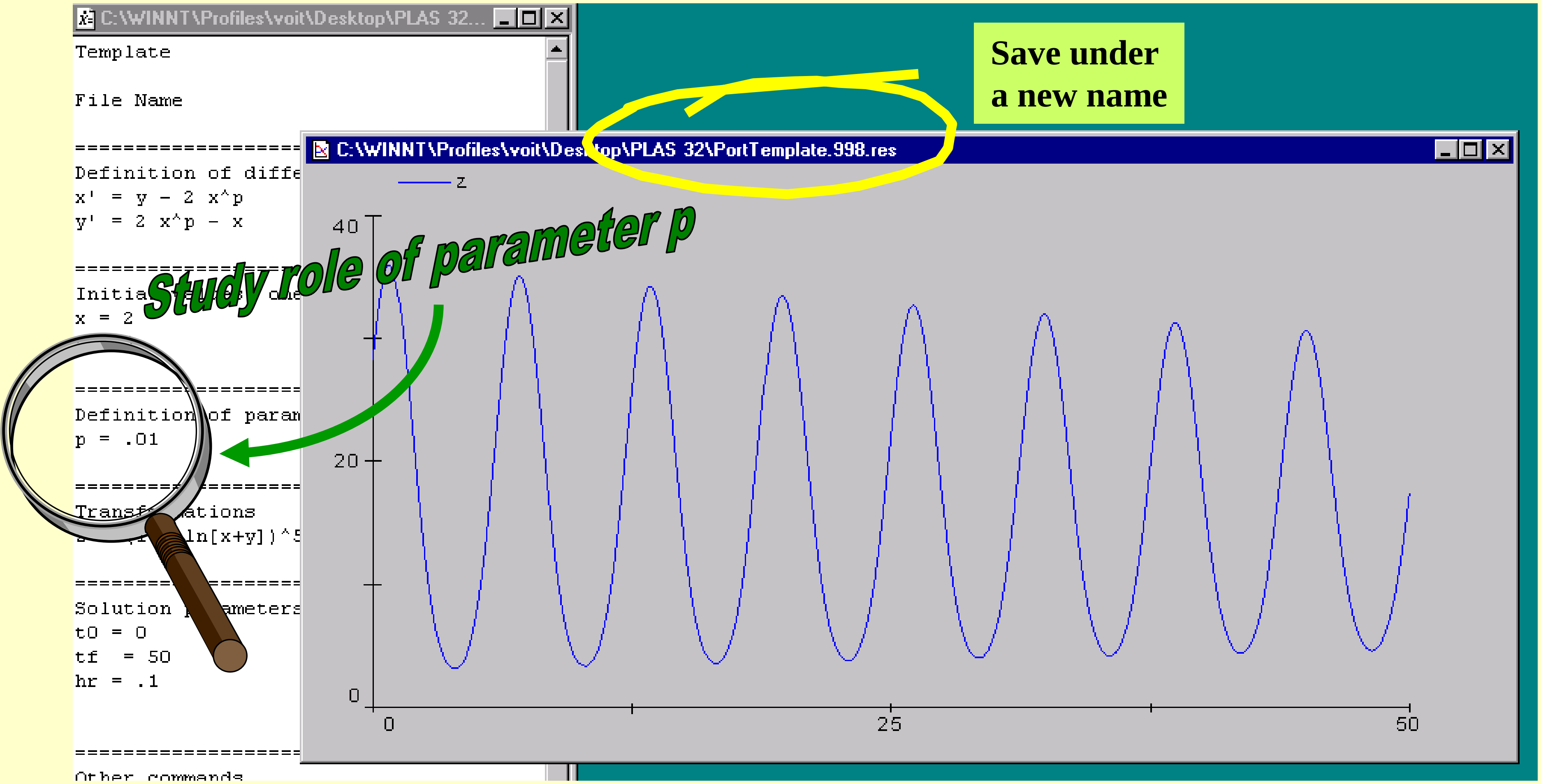
Display of Steady-State Features (ẋ=0)



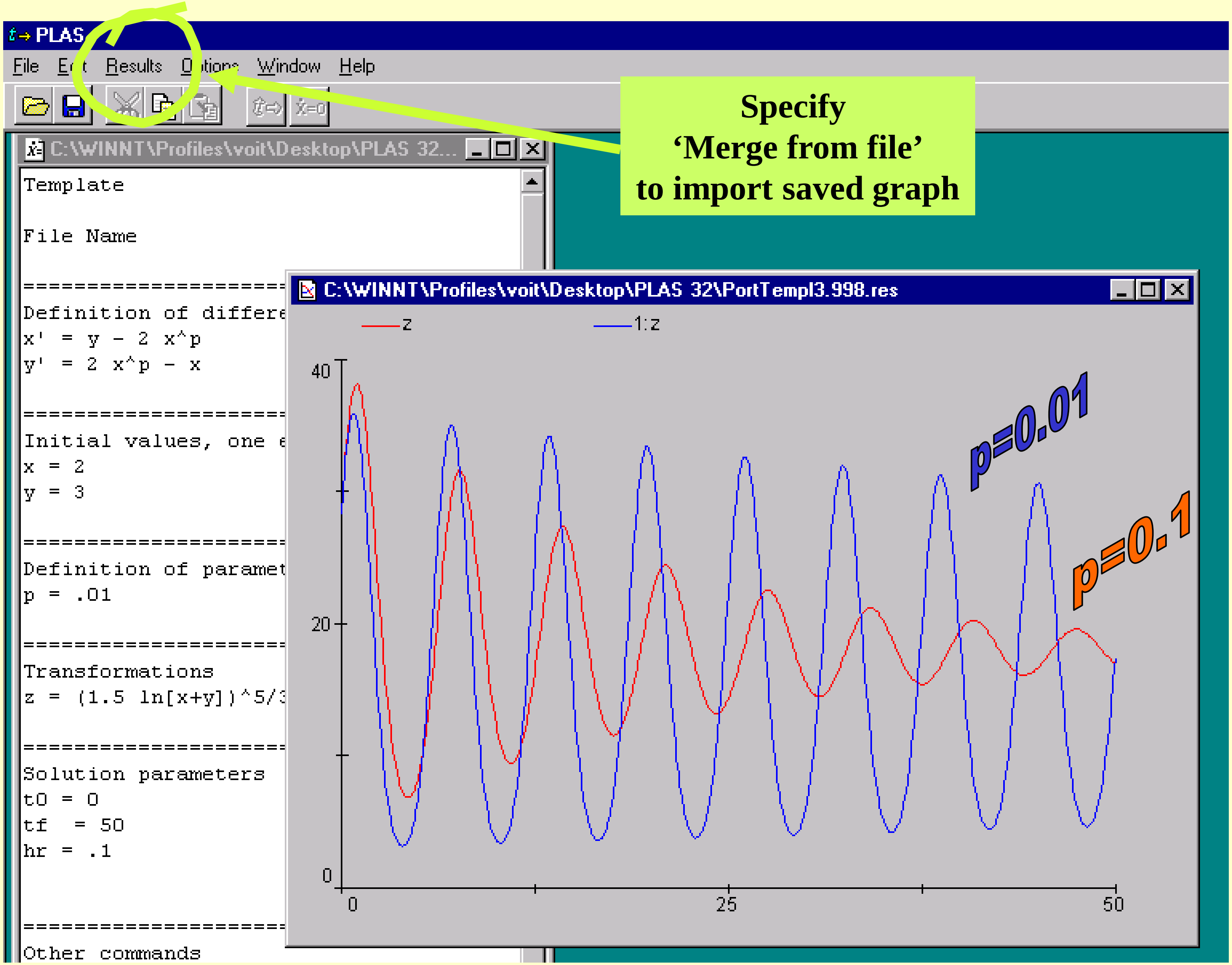
Display of Variable Sensitivities



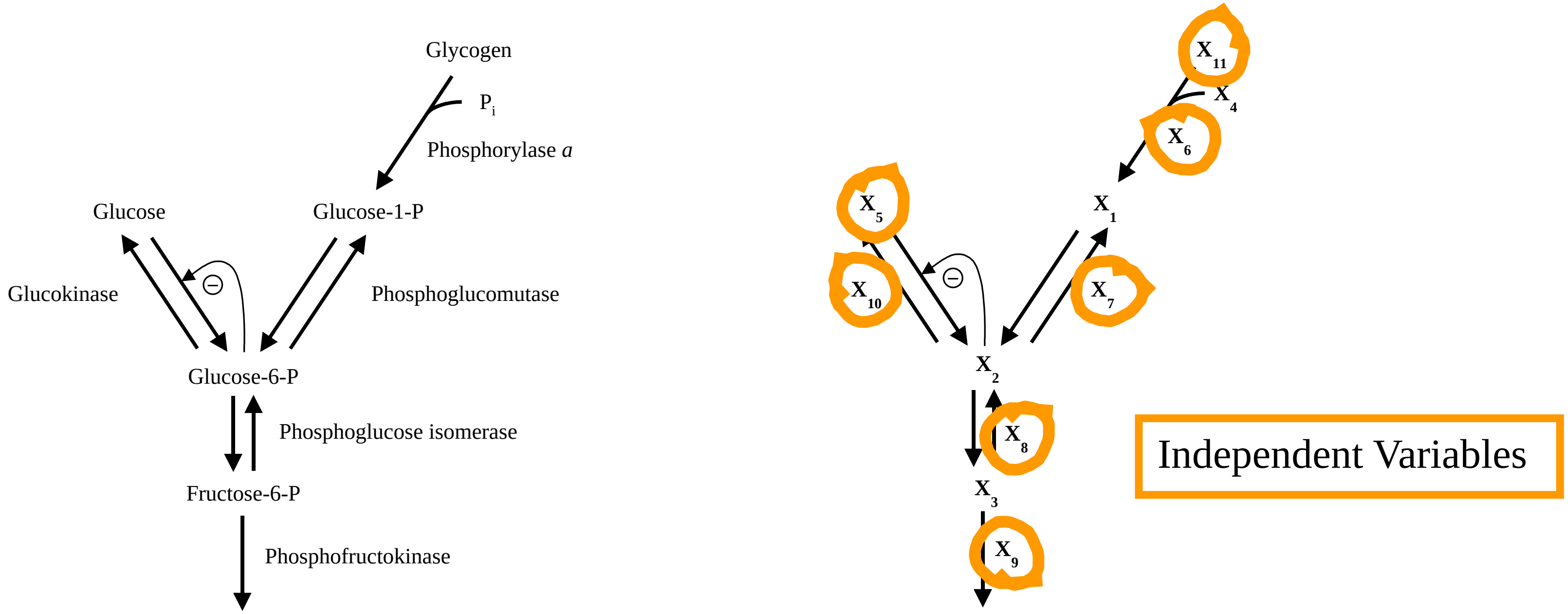
Comparative Simulation Studies



Comparative Simulation Studies (Cont'd)



Example: Initial Steps of Glycolysis and Glycogenolysis*



GMA Model

$$\dot{X}_1 = 0.077884314\, X_4^{0.66} X_6 - 1.062708258\, X_1^{1.53} X_2^{-0.59} X_7$$

$$\dot{X}_2 = 0.585012402\, X_1^{0.95} X_2^{-0.41} X_5^{0.32} X_7^{0.62} X_{10}^{0.38} - 7.93456 \times 10^{-4} X_2^{3.97} X_3^{-3.06} X_8$$

$$\dot{X}_3 = 7.93456 \times 10^{-4} X_2^{3.97} X_3^{-3.06} X_8 - 1.05880847\, X_3^{0.3} X_9$$

* 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 (Cascante 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
```

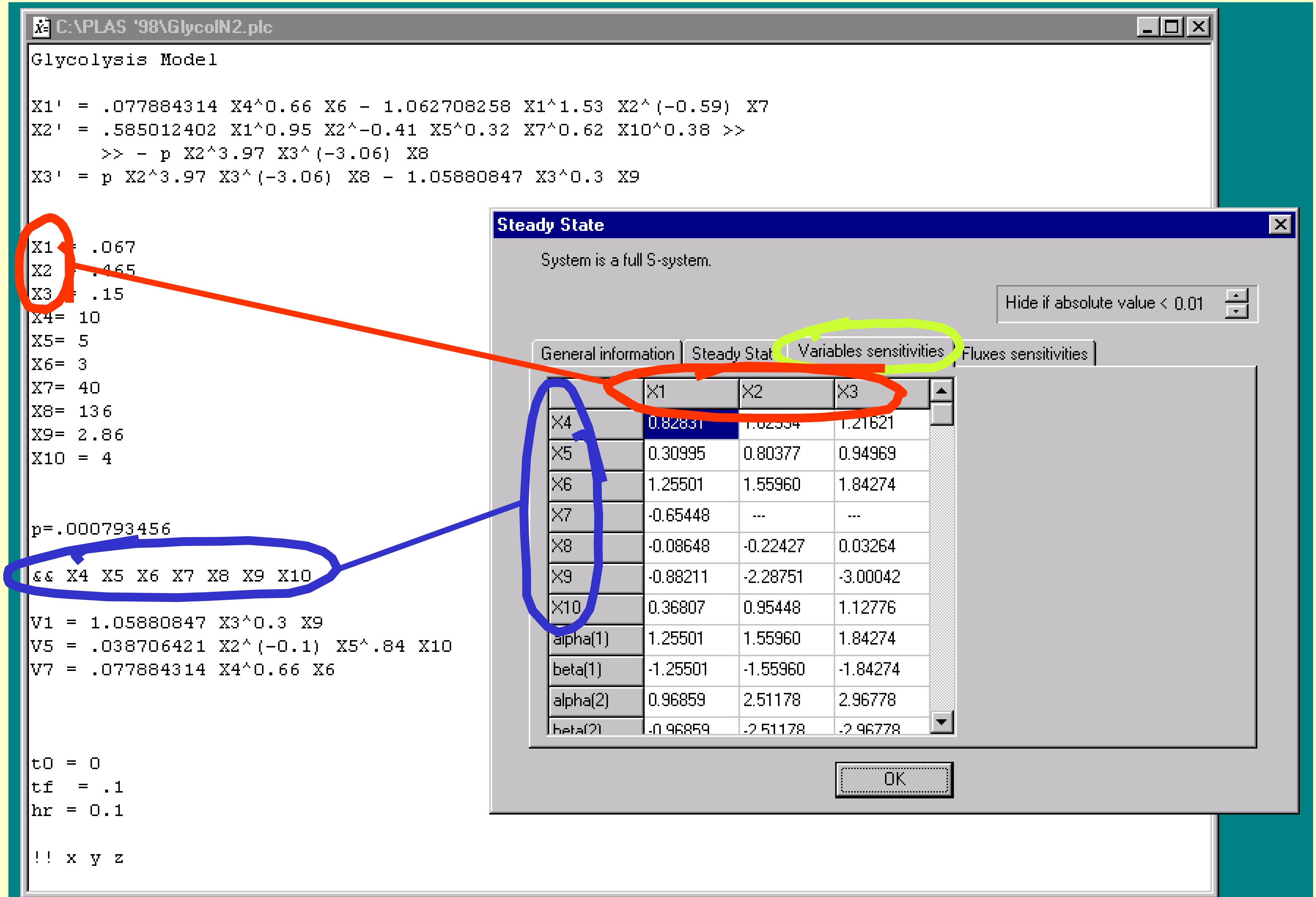
Continuation Symbol

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 = .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
```

Steady State

System is a full S-system.

Hide if absolute value < 0.01

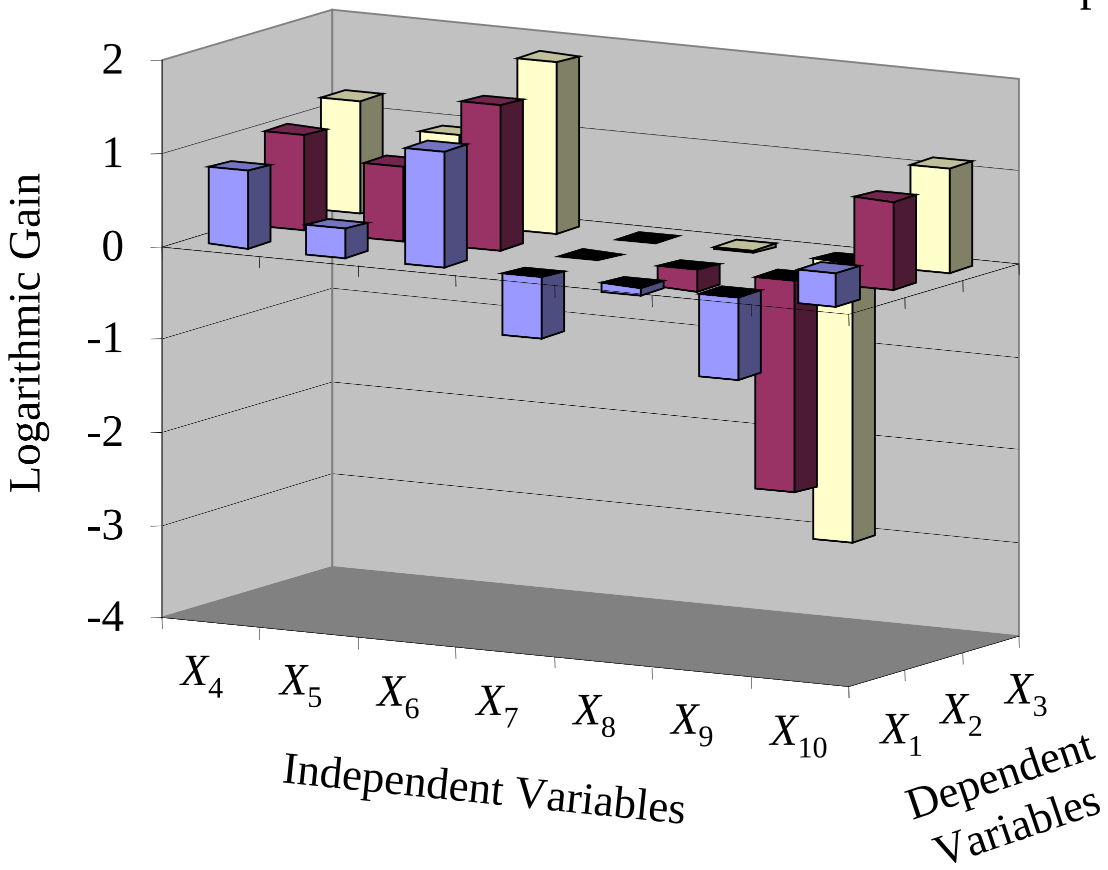
General information | Steady State | Variables sensitivities | Fluxes sensitivities

	X1	X2	X3
X4	0.82831	1.02354	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

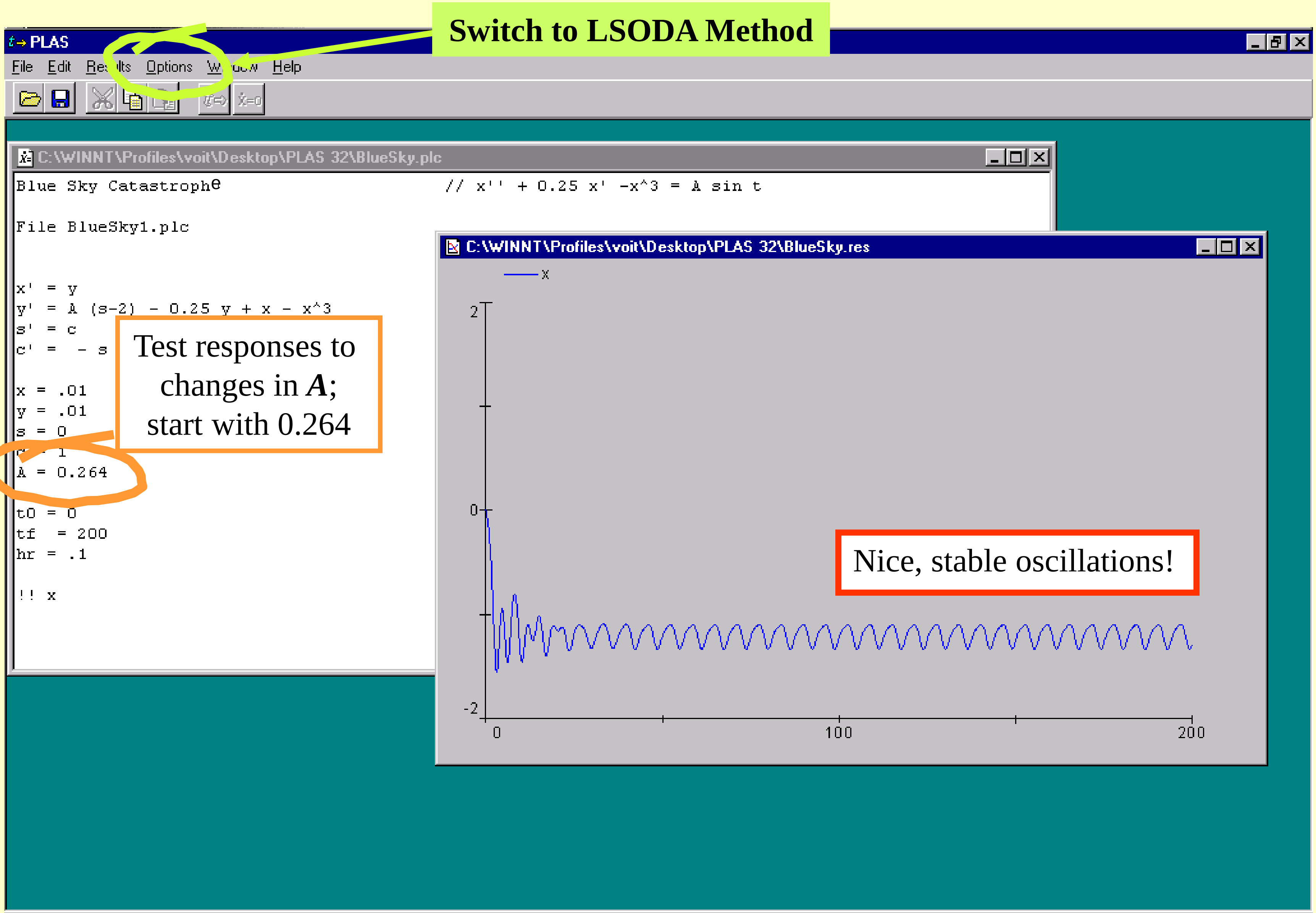


Dynamics:
Blue Sky Catastrophe
(see Chapter 2)

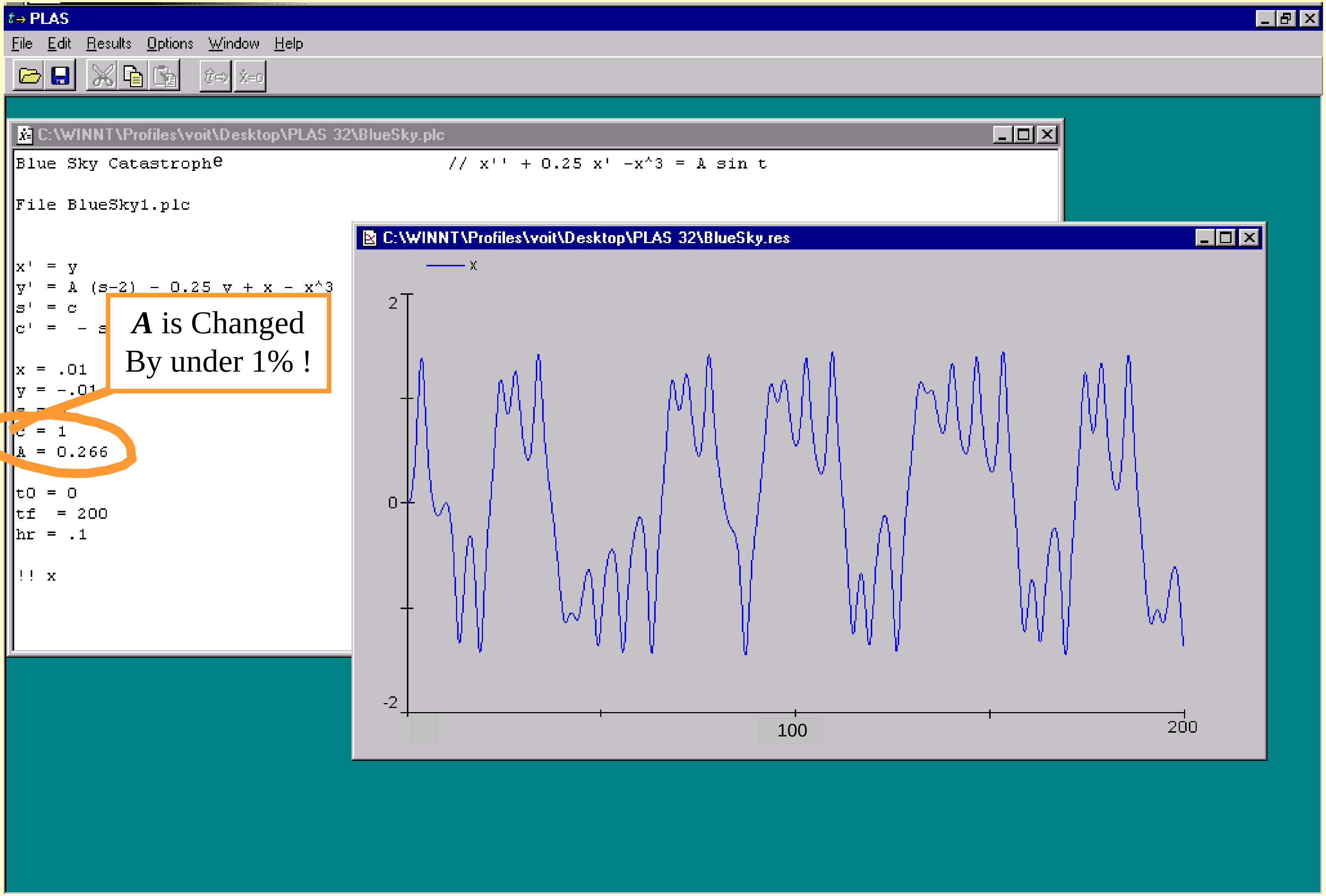
C:\WINNT\Profiles\voit\Desktop\PLAS 32\BlueSky.plc

```
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
```

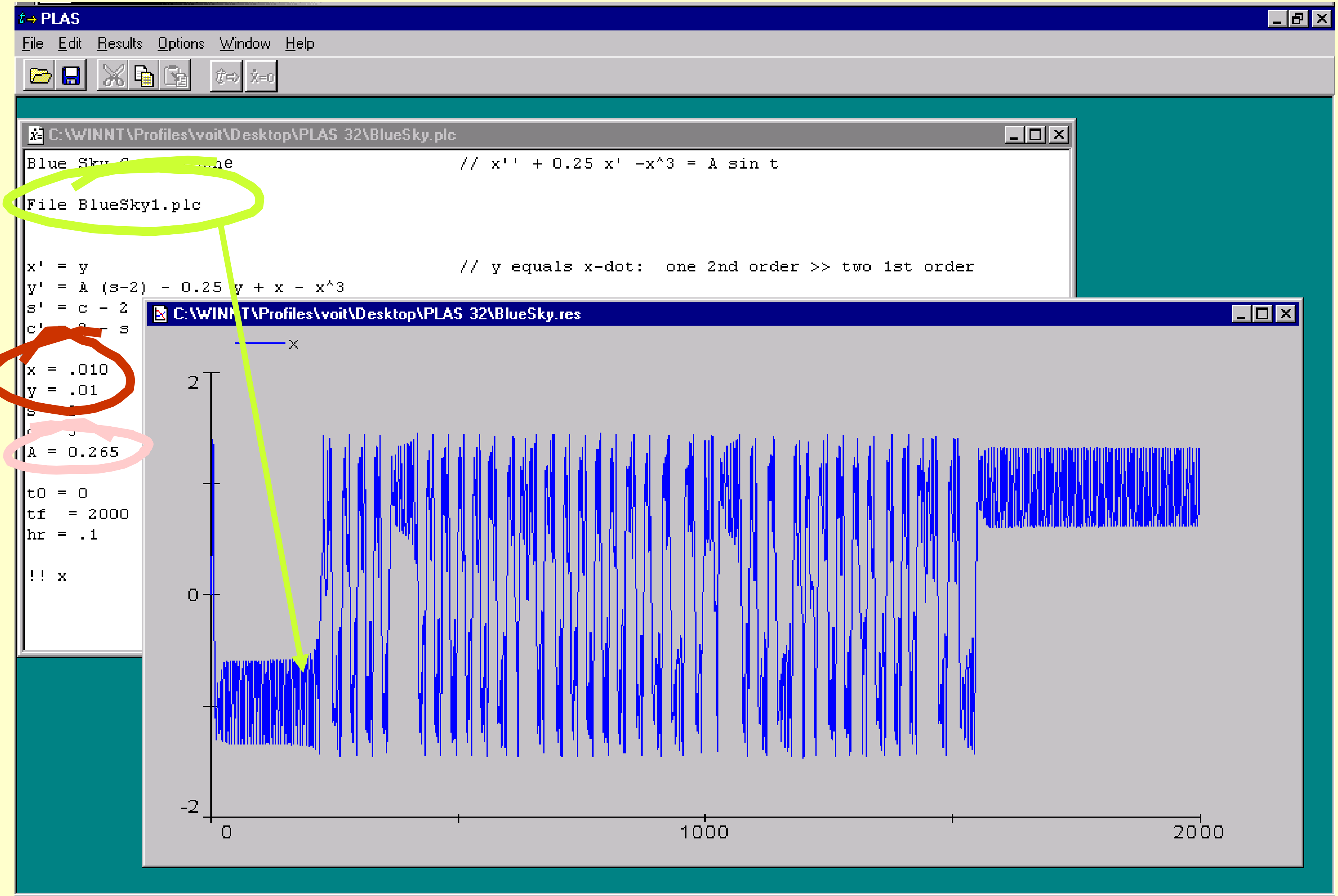
Use of LSODA Solver for Stiff or Non-Power-Law Systems



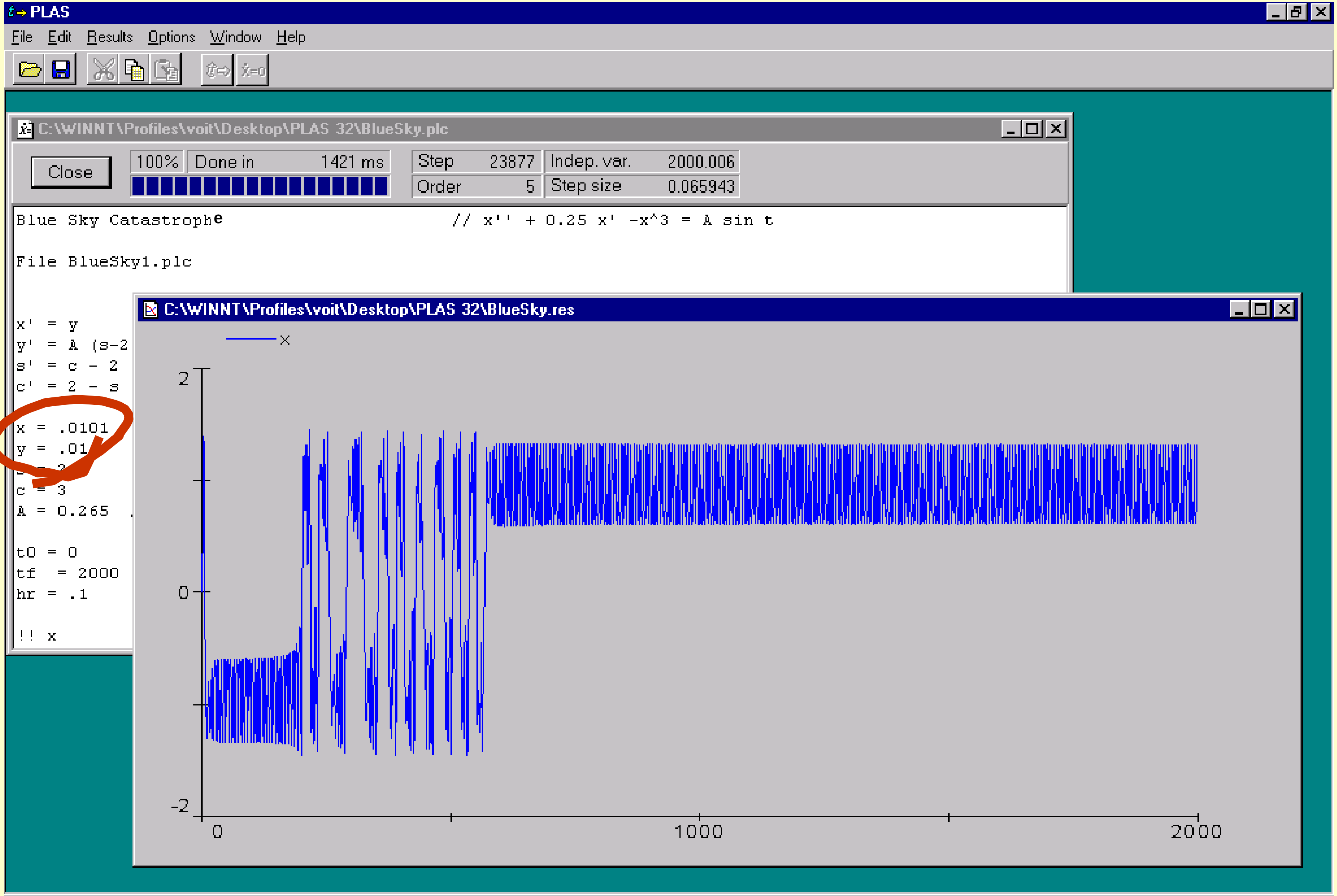
Dynamics is Extremely Sensitive to Changes in Parameter *A*



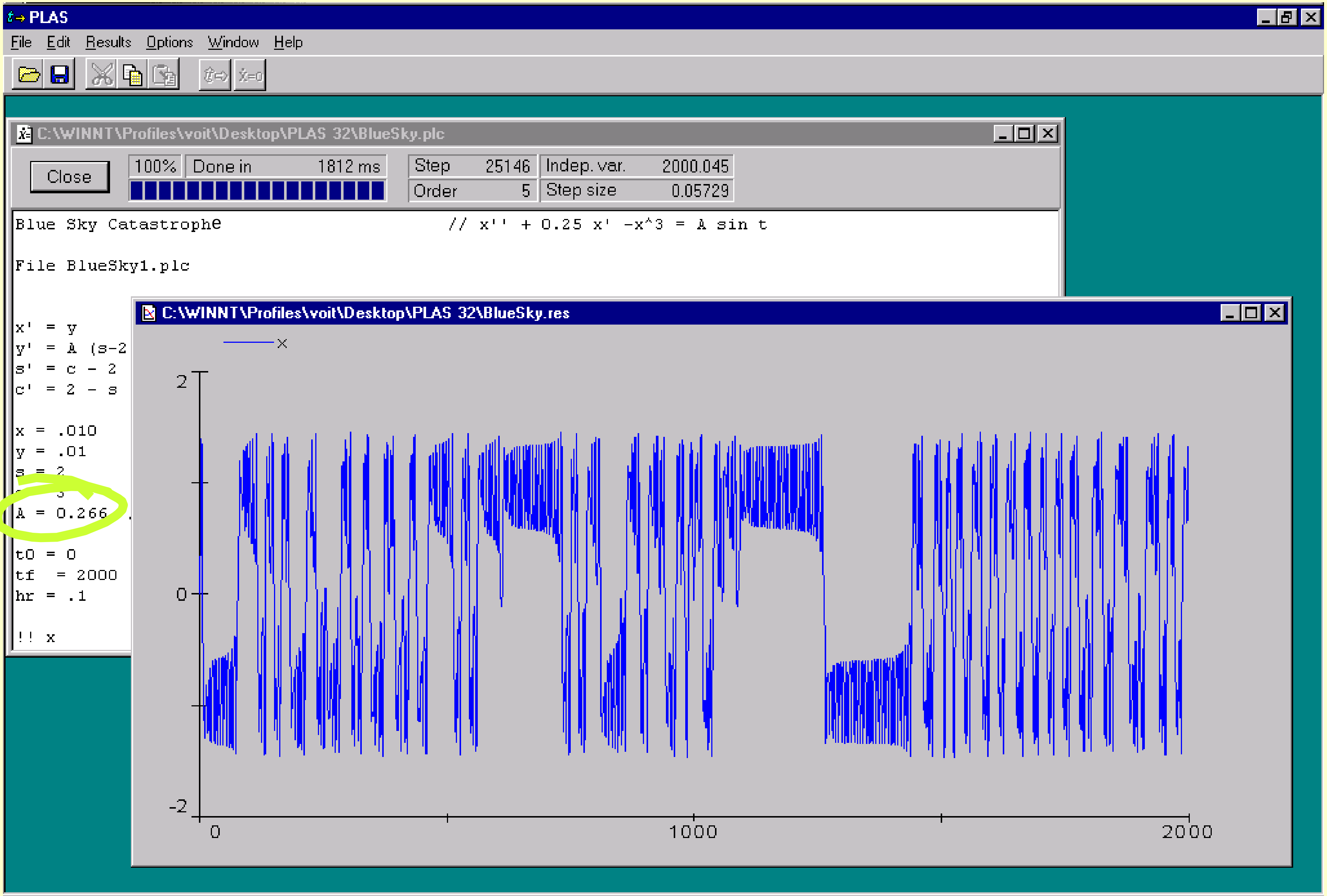
Dynamics is Extremely Sensitive to Changes in Initial Values



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

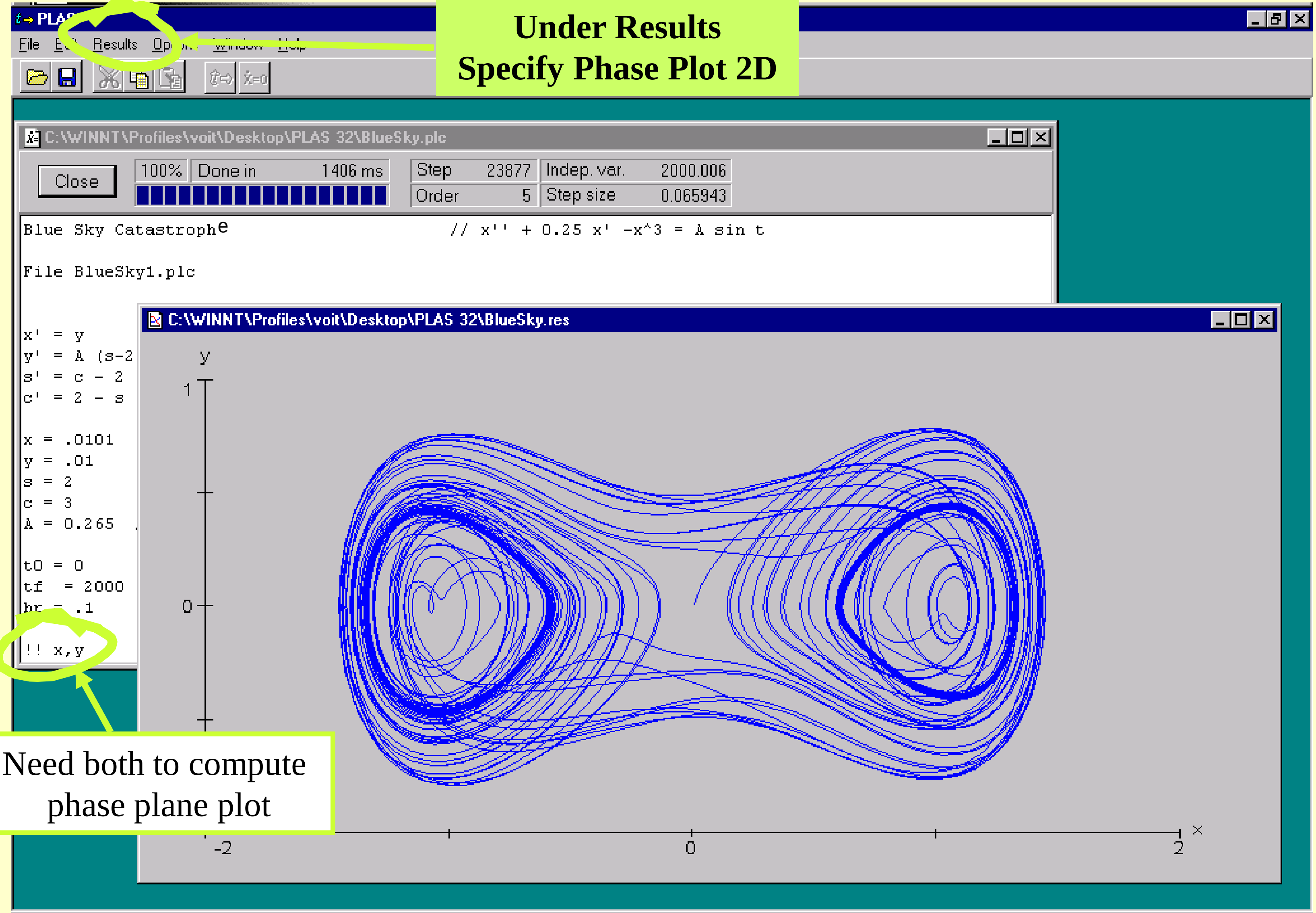


Chaotic Dynamics is Extremely Sensitive (cont'd)



Phase-Plane Plot of Chaotic System

Under Results
Specify Phase Plot 2D



Need both to compute phase plane plot

Pseudo-3D Plot of the Chaotic System

```
x' = y
y' = A (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

A = 0.265

!! x y t
```

Create explicit variable for time (scaled)

Pseudo-3D Plot of the Chaotic System