RK4

Version 3.0

(updated 12/1/2006)

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Description: An Excel add-in to produce an **Excel** spreadsheet that renders a fixed-interval, fourth-order Runge Kutta method for solving initial value systems for small to medium-size simulation studies.

Rationale: **Excel** spreadsheets are familiar to several PC users. Once rendered, the spreadsheets will contain formulas which the user can later modify using standard **Excel** commands or enhanced/advanced commands based on other add-ins such as **SOLVER** to perform further analysis or parameter estimation.

Special Features:

1. Ability to easily attach scroll bars to chosen parameters and initial conditions. This allows the user a quicker interface to perform simulation studies.
2. Ability to open and save model files (the default file extensions are *.rk4). These files are ordinary text files. Thus, they can be also be created and edited using any text editor such as **NOTEPAD** or **WORDPAD**.
3. A simple interface for generating several time-plots or phase plane plots.
4. A simple interface to obtain parameter estimation of models based on combining several data sets. The data sets can have different and non-uniform sampling points.

Installing the RK4 Add-In:

1. Save the file: **rungekutta4_v3.xla** in a directory which is relatively permanent.
2. Open the Excel program and make sure at least one workbook is open.
3. Pull-down the [**TOOLS**] menu and select [**ADD-INS...**] submenu item. The ADD-INS window should pop out .)
4. Click the [**BROWSE...**] button, then open the file: **rungekutta4_v3.xla**
5. Click the [**OK**] button. (This should activate the **RK4** add-in and a command bar should appear on the upper left corner as shown in Figure 1.)
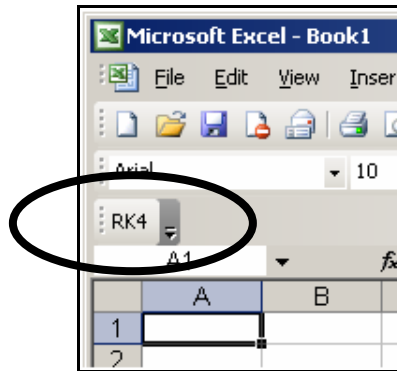

Figure 1. The RK4 Command Bar

Activating/Deactivating RK4:

1. Pull-down the [**TOOLS**] menu and select [**ADD-INS...**] submenu item. (The ADD-INS window should pop out.)
2. Click on box next to the [**Rungekutta4_v3**] item. A check indicates activation while removing the check will deactivate **RK4**.
3. Click on [**OK**] button. If **RK4** is activated, the command bar shown in Figure 1 should appear.

Uninstalling the RK4 Add-In:

1. First deactivate the **RK4** add-in as discussed above.
2. Delete the file: **rungekutta4_v3.xla** (Alternatively, you could the move the file to a different directory or rename it.)
3. Next, go to [**TOOLS**]→[**ADD-INS...**] submenu. Try activating the **RK4** add-in by clicking on the checkbox.
4. A window should pop-out asking "**Cannot find add-in… Delete from list ?**" Click on the [**Yes**] button.
5. Click [**OK**] on the ADD-INS window. **RK4** should then be uninstalled. (To reinstall, go to installing instructions given above.)

Removing the RK4 Toolbar (for MS Excel 2003):

1. Right-click on the [**RK4**]-toolbar option button (down-arrow on the right of the button), and then select [**Add or Remove Button**]→[**Customize**] menu. (see Figure 1a).
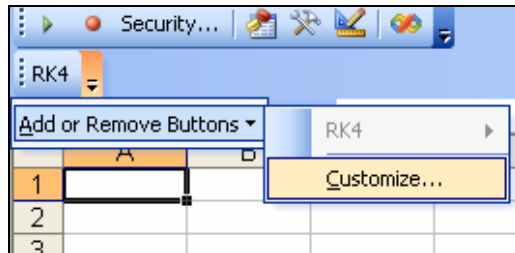

Figure 1a.

2. A new window should appear (see Figure 1b). Under the [**Toolbars**] – tab, drag the scrollbar all the way down and select [**RK4**]. The check-mark will not change, but the [**Delete**] button should become enabled. Click [**Delete**] and click [**OK**] when prompted. Then click on [**Close**] to exit the Customize window. (Note: if **RK4** had not been uninstalled according to procedure above, then the **RK4** toolbar will not be permanently removed.)
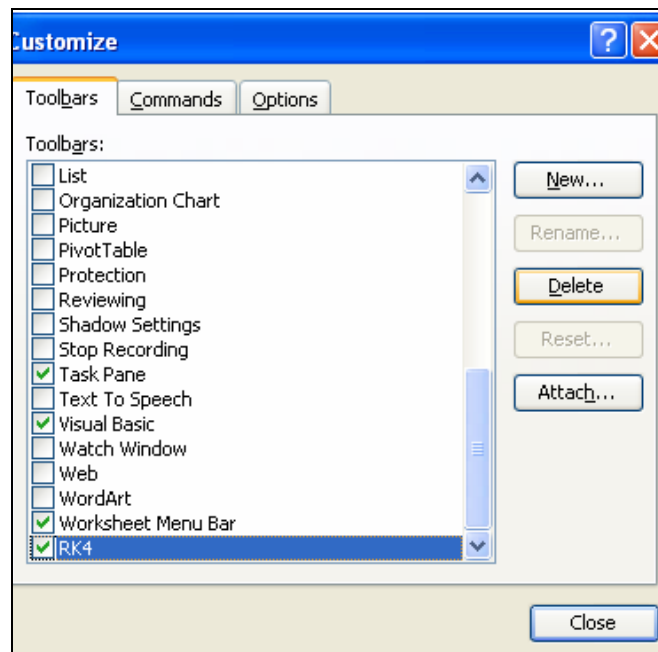

Figure 1b.

Tutorial:

(We recommend strictly following the example inputs in the tutorials including the intentional errors. This way, one could observe the different responses of the add-in program, and learn how to recover from and correct the errors.)

Variables and Parameters:

Before we begin with the applications, a few rules need to be clarified:

1) "State variables" are variables that are defined with derivatives.
2) "Other variables" are variables that are obtained from algebraic equations. (Please avoid algebraic loops.)
3) Both "State variables" and "Other variables" need to be enclosed by square brackets, e.g. [x], [T_cool], etc.
4) "Parameters" are numbers that will be varied per simulation to observe its effects on the process. To distinguish "Parameters" from either "State variables" or "Other variables", do not enclose by square brackets.
5) The time variable will be given a special notation: [t]. So, do not use [t] as a member of "State variable" or "Other variable".

The examples below will illustrate implementations of these rules.

The following files are needed (available from the distribution files) for the following tutorials:

        Application 2:   **Application_2_code.rk4**
        Application 3:   **Application_3_code.rk4**, **iodata.dat**
        Application 4:   **Application_4_code.rk4**, **Circle.ics**
        Application 5:   **Application_5_code.rk4**, **case1.dat**, **case2.dat**

Application I: Using RK4 interface to input model directly.

Recommended use: when the number of variables and parameters are relatively small.

Example Scenario:

A controlled process described by

$$\frac{dT}{dt} = \frac{T_{in} - T}{\tau} + u$$

$$T(0) = 5.0$$

where

$$T_{in} = 1 - \frac{1}{2}\exp(-2t)$$
$$u = K_c\left(T_{set} - T\right)$$

with parameters,

$$T_{set} = 20$$
$$0 \le K_c \le 10 \quad (\text{Nominal value}:1.0)$$
$$1 \le \tau \le 5 \quad (\text{Nominal value}:3.0)$$

We want to simulate this process from $t = 0$ to $t = 20$ at fixed intervals $\Delta t = 0.1$. In addition, we want to observe the behavior for initial conditions of T ranging from 0 to 10.

Example Session:

1. Click on RK4 button in the command bar (see Figure 1.). A user interface window as shown in Figure 2 should pop out.

Figure 2. RK4 Input Window.

2. Select the [**Initialization**] folder tab and enter the values for time interval and final time. (Make sure that the [**Regular**] option is selected.)
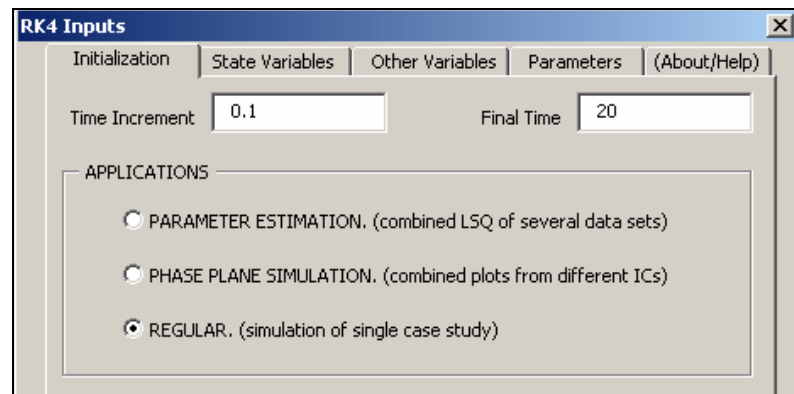

Figure 3. Time Setting Folder Tab.

3. Next, select the [**State Variables**] folder tab and input the information as shown in Figure 4. (You can use the <ENTER> key or sometimes the <TAB> key to move the focus to the next input prompts.)
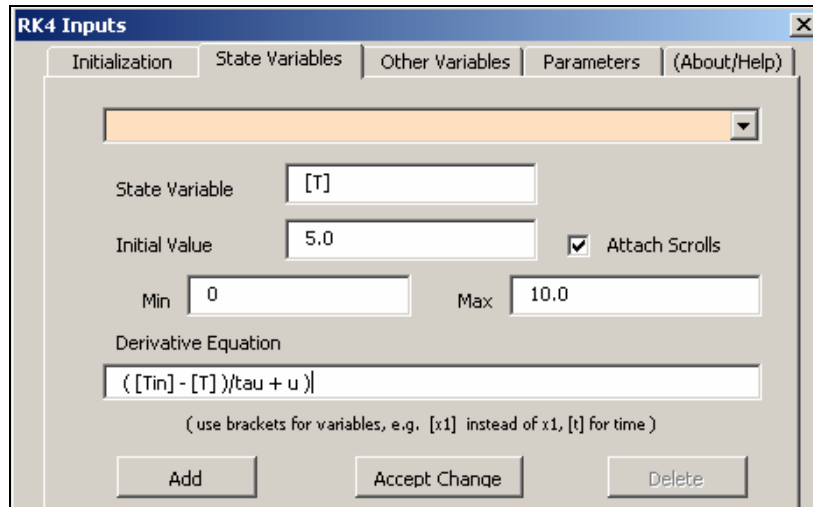
Figure 4. STATE VARIABLES Folder Tab.

Note: put the extra left parenthesis as shown in Figure 4 as an intentional error. Then click the [**Add**] button. A warning should pop out to warn of a parenthesis mismatch error.
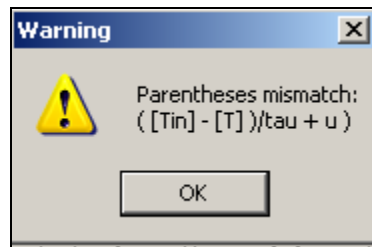

Figure 5. Parenthesis-Mismatch Warning Window.

Click [**OK**] to acknowledge the warning. Then manually remove the extra rightmost parentheses.

4. Click on the [**Add**] button to accept the corrected inputs.

Note that T_{in} needs to be enclosed with square brackets because it is a variable rather than a parameter. The same should be true for u. However, we will continue with this intentional error to see how the RK4 program will respond to this situation.

5. Next, switch to the [**Other Variables**] tab folder and input the equations for variables that are not state variables. Figure 6 shows the input for T_{in} .
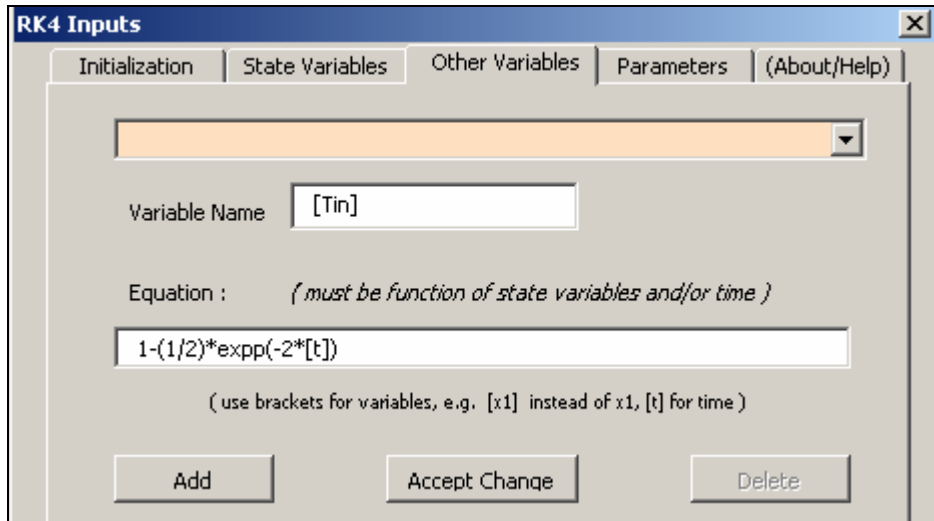
Figure 6. OTHER VARIABLES Folder Tab.

The time variable is entered as [t]. Because RK4 is case-sensitive, this will not be confused with [T] used for our state variable.

Note again another intentional error for the function exp which was misspelled with an extra letter "p". We will see later how RK4 will respond to this type of error.

Click the [**Add**] button and continue with entering the equation for *u* as shown in Figure 7.
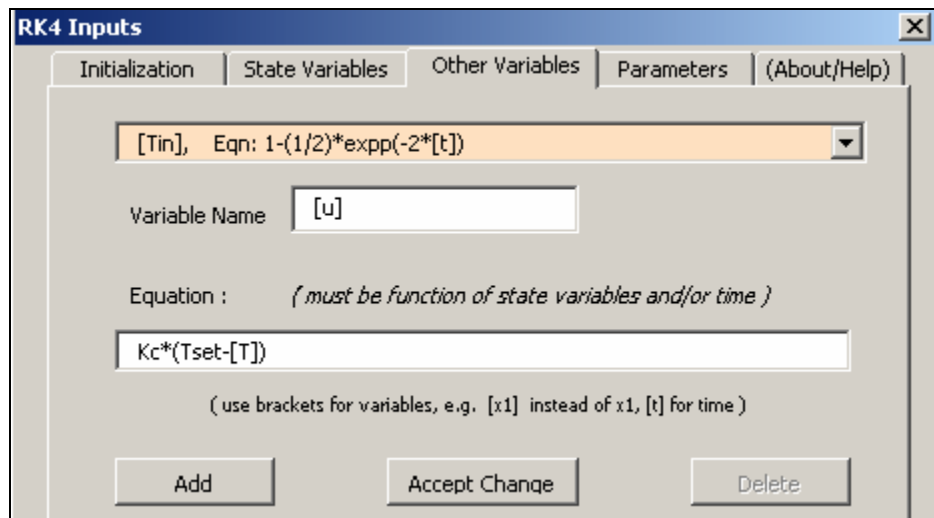

Figure 7. Adding information for *u*.

Click the [**Add**] button to accept the entries.

6. Next, select the [**Parameters**] tab and enter the information shown in Figures 8 to 10. (Note: The [**Accept Change**] button replaces the current variable, while [**Add**] simply adds the current variable to the list.)

Figure 8. [**Parameters**] Folder Tab

Figure 9. Attaching Scroll Values to Parameter K_c.

The [**Min**] and [**Max**] input prompts will appear after checking the [**Attach Scrolls**] option.

Figure 10. Attaching Scroll Values to Parameter τ.

7. Once all the input information has been keyed in, click on the [**OK**] button on the bottom of the RK4 Input Window.

8. Because we forgot to include the brackets for the variable *u* earlier, the program is assuming that *u* was a parameter. An error window as shown in Figure 11 should pop up on the right to list missing (undefined) and repeated variables and parameters.
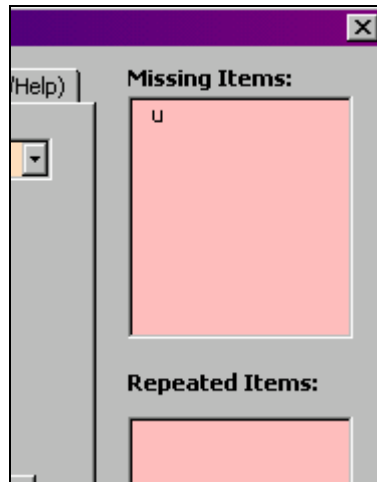

Figure 11. Error Windows.

9. To correct this error, go back and select the [**State Variables**] folder tab. In the combo-list window (yellow window), select the entry for [T].

   Double-click on the yellow window. The entries should show in the appropriate input boxes.

   Include square brackets around *u*, then click on the [**Accept Change**] button as shown in Figure 12.
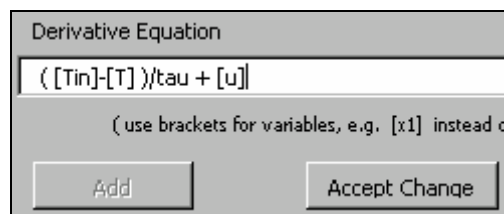

Figure 12. Editing Derivative Equation.

10. Click on the OK button again.

This time the error window should contain the location of function errors. (RK4 will accept any functions of numeric arguments that the current Excel session allows, including additional functions introduced by other add-ins.)
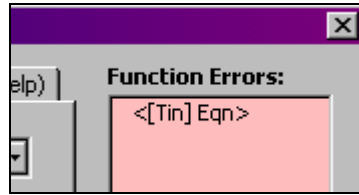

Figure 13. Error Window Showing Location of Function Errors.

Edit the entry for [Tin] and correct the function "expp" by removing the extra letter "p".

11. Click OK one more time. Since no RK4-predictable error is found, a "Last Chance To Save" warning will pop out to allow the saving of the various inputs into a text file for easier recovery in the future. (The file is recommended to have the extension *.rk4, but this is not necessary.)

The RK4 Input Window will disappear.

The simulation will then be processed by the program to yield an Excel spreadsheet with the required inputs and formulas in the appropriate cells as shown in Figure 14.

	A	B	C	D	E	F	G	H	I
1									
2		dt	0.1						
3		Final t:	20						
4	Parameters:	Tset:	20						
5		Kc:	1		Min:	0	Max:	10	
6		tau:	3		Min:	1	Max:	5	
7	Initial Values:	[T]:	5		Min:	0	Max:	10	
8	Derivatives:	d[T]/dt=	([Tin] - [T])/tau + [u]						
9	Algebraic Eqns:	[Tin]=	1-(1/2)*exp(-2*[t])						
10		[u]=	Kc*(Tset-[T])						
11									
12									
13	dt	Time	[T]	[Tin]	[u]	d1,1	d2,1	d3,1	d4,1
14		0	5	0.5	15	1.35	1.261586	1.26748	1.184024
15	0.1	0.1	6.265359	0.590635	13.73464	1.184307	1.106651	1.111828	1.038536
16	0.1	0.2	7.375326	0.66484	12.62467	1.038784	0.970595	0.975141	0.910791
17	0.1	0.3	8.348835	0.725594	11.65117	0.911009	0.851145	0.855136	0.798648

Figure 14. Spreadsheet Rendered by RK4.

The RK4 command bar should also have changed. The RK4 button will be replaced by a PLOT button.

The scrollbars can now be used to change parameter values and initial values. The maximum and minimum values attached to the scroll bars can be changed manually in the spreadsheet.

(Caution: we discourage direct editing of parameters or initial values that are attached to scrollbars since this will disable the formula links to the scrollbars. In case you did input a value directly, or have accidentally done so, you could still recover the scrollbar formula manually. For example, the formula for cell C5 is given by: "= F5 +D5 *(H5-F5)/50" where the number 50 is fixed since the scrollbar was programmed to have 50 fixed incremental changes.)

One could check that the formulas for the cells in the solution block are simply those translated from the model under the fourth-order Runge-Kutta method.

12. Click on the PLOT button in the toolbar. A window should pop out (see Figure 15). Select the variables in the x-axis and the y-axis. Turning on the "Freeze Scales" checkbox will disable the automatic rescaling of the axes. This is particularly useful when you want to observe how the plot changes accordingly with the changes in the parameter and initial values, specially via the scrollbars.
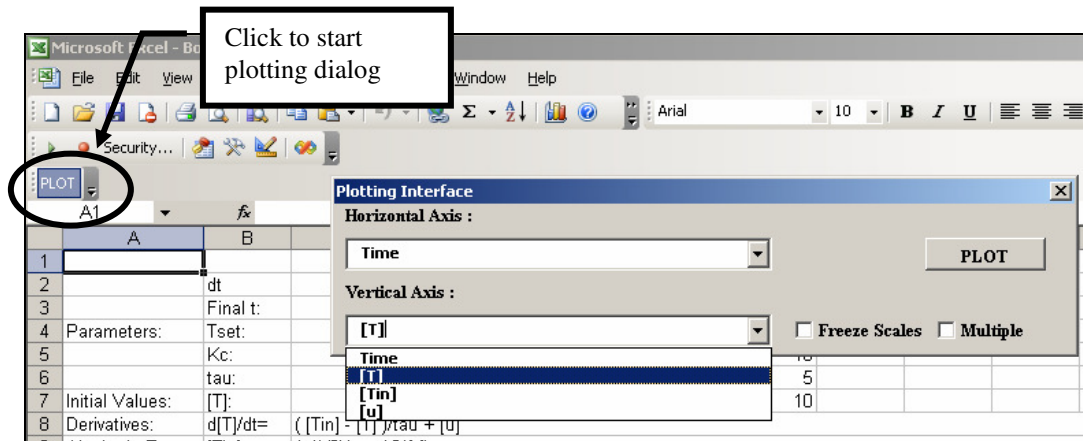
Figure 15. Plotting dialog

Notes:

i) The plots are generated by Excel statements and thus can be changed by the usual procedures in Excel.

ii) One can keep clicking the PLOT button to create several plots.

iii) By changing the parameters values (specially through the scroll bars) one can see how the different plots change accordingly.

iv) One can also move any of the plots to be a separate chart for printing out individual charts.

Application II. Using a text editor to create/edit RK4 model file.

Recommended use: when the number of variables and parameters are much larger and thus easier to introduce using a text editor.

Example Scenario:

A PI-controlled second order process described by

$$\frac{dx_1}{dt} = x_2$$

$$\frac{dx_2}{dt} = \frac{1}{\tau_n^2}\left(-2\tau_n\,\zeta\,x_2 - x_1 + u\right)$$

$$x_1(0) = 1.0 \quad ; \quad x_2(0) = 0$$

$$P = x_1$$

where,

$$u = K_c\left[\left(P_{set} - x_1\right) - \frac{1}{\tau_I}e_{int}\right]$$

$$\frac{d\,e_{int}}{dt} = P_{set} - x_1$$

$$e_{int}(0) = 0$$

with parameters,

$$P_{set} = 2.0$$

$$0 \le K_c \le 20 \qquad \text{(Nominal value:1)}$$

$$0.2 \le \tau_I \le 5 \qquad \text{(Nominal value:5)}$$

$$1 \le \tau_n \le 5 \qquad \text{(Nominal value:1)}$$

$$0 \le \zeta \le 1 \qquad \text{(Nominal value:0.5)}$$

We want to simulate from $t=0$ to $t=20$ with $\Delta t=0.1$.

Example Session:

1. Using a text editor, e.g. NOTEPAD (or MS WORD but later saving the file as a text file), input or copy-and-paste the lines shown in Figure 16 and save the text file.

```
'
' Second Order Process with PI Control
' ====================================
'


' Time Settings
' -------------

    dt:    0.1
    tfinal: 20

' State Variables
' ---------------

    [x1], Initial Value: 1,  Deriv:[x2],          Min: 0.,       Max: 2
    [x2], Initial Value: 0,  Deriv:(1/taun^2)*(-2*zeta*taun*[x2]-[x1]+[u])

    [P],  Eqn:[x1]  ' output pressure is given by [x1]

'
' PI controller
' -------------

    [u],    Eqn: kc*( (Pset-[x1]) + [eint]/taui )
    [e],    Eqn: Pset-[x1]
    [eint], Initial Value: 0,    Deriv: Pset-[x1]

' Parameters
' ----------

    Pset,   Value: 2.0
    kc,     Value: 1.0,    Min: 0,    Max: 20
    taui,   Value: 5,      Min: 0.2,  Max: 5
    taun,   Value: 1.0,    Min: 1,    Max: 5.0
    zeta,   Value: 0.5,    Min: 0,    Max: 1
```

Figure 16. Code for Input Model of 2nd Order System with PI Control.

A simple set of rules applies to coding of the model:

a) The characters following a single quote symbol (') in a single line are treated as comments and will be ignored by RK4.
b) Blank spaces, blank lines and <TABS> will also be ignored. Use these to make the file readable.
c) The lines can be in any order.
d) For state variables, the syntax is given by:

> *stateVarName*, Initial Value: *initval*, Deriv: *derivEqn*, Min: *minval*, Max: *maxval*

> *Example:* [x1], Initial Value: 1, Deriv:[x2], Min:0, Max:2

"Initial Value:" and "Deriv:" are required key phrases. "Min:" and "Max:" are needed if scrolls are going to be attached to the state variable for minimum or maximum range of initial values, otherwise you can leave them out. The commas are also the required delimiters. If no scrolls are needed, do not put a comma after the derivative equation.

The sequence within the line should also be strictly followed. Do not break the line with a carriage return or line feed. (If NOTEPAD is used, it is recommended to disable word-wrapping option.)

e) For other variables, the syntax is given by:

otherVarName, Eqn: *algebraicEqn*

Example: `[u], Eqn: kc*( (Pset-[x1]) + [eint]/taui )`

"Eqn:" is a required keyword. The commas are the required delimiters. The sequence within the line should also be strictly followed. As before, do not break the line.

f) For parameters, the syntax is given by:

parameterName, Value: *parameterValue*

Example: `Pset, Value: 2.0`

"Value:" is a required keyword. As before, commas are needed delimiters and the lines should not be broken.

For parameters with attached scrolls, append the "Max:" and "Min:" keywords.

parameterName, Value: *parameterValue,* Min: *minValue,* Max: *maxValue*

Example: `taun, Value: 1.0, Min: 1, Max: 5.0`

2. Open the Excel spreadsheet with RK4 activated.

3. Click on the RK4 button in the command bar.

4. Click on the OPEN button in the RK4 Input Window.

5. Open the file containing the model code. An "APPEND or REPLACE" window should appear as shown in Figure 17. Click YES to append or NO to erase current contents and replace them with contents from the openned file.
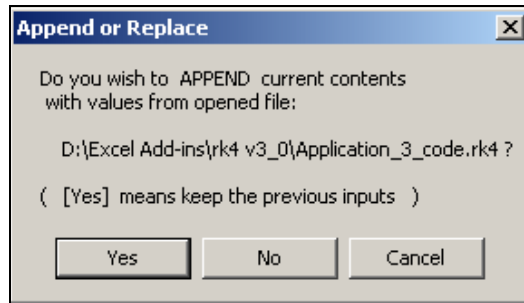
Figure 17. Choice Window for Appending or Replacing Contents.

6. Proceed as before in Application I, i.e. edit any existing errors and click OK to proceed to spreadsheet rendering.

Application III. Using Solver with RK4 Worksheets.

Recommended use: when optimizing parameters and initial conditions for purposes of parameter estimation or other application such as controller tuning.

Example Scenario:

Given the set of input-output data obtained at uniform sampling intervals of 0.1 (data included as a text file, iodata.dat). whose plots are shown in Figure 18. (Note that the output data contains noise.)
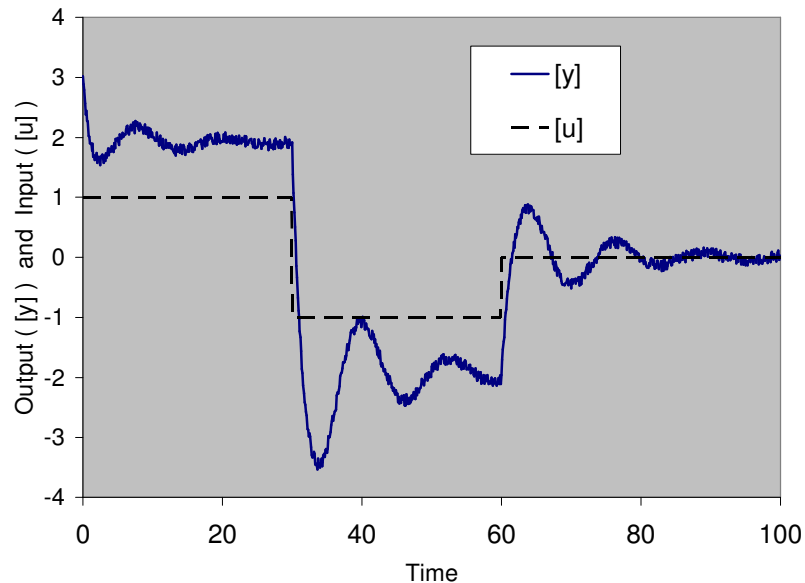
Figure 18. Data used for parameter estimation example.

Suppose we want to determine a third-order linear model that fits the data based on the least-squared-error criteria, i.e. we want to determine the parameters a_0, a_1, a_2, b_0, b_1 and b_2 in the following linear dynamic model:

$$\frac{dx_1}{dt} = -a_2 x_1 + x_2 + b_2 u$$

$$\frac{dx_2}{dt} = -a_1 x_1 + x_3 + b_1 u$$

$$\frac{dx_3}{dt} = -a_0 x_1 + b_0 u$$

$$y = x_1$$

Example Session:

> Use RK4 to obtain a spreadsheet based on initial guess on parameters and initial conditions. For instance, open the code shown in Figure 19 with RK4 to produce the spreadsheet shown in Figure 20.

```
'
' Sampling interval and final time
' --------------------------------
'
dt: 0.1
tfinal: 100
'
' State Equations
' ---------------
'
[x1],    Initial Value: 3,    Deriv:-a2*[x1]+[x2]+b2*[u]
[x2],    Initial Value: 1,    Deriv:-a1*[x1]+[x3]+b1*[u]
[x3],    Initial Value: 1,    Deriv:-a0*[x1]+b0*[u]
'
' Input Variable
' --------------
'
[u],     Initial Value: 1,    Deriv:0
'
' output Variable
' --------------
'
[y],    Eqn: [x1]
'
' Parameters
' ----------
'
a2,    Value: 1
a1,    Value: 1
a0,    Value: 1
b2,    Value: 1
b1,    Value: 1
b0,    Value: 1
```

Figure 19. RK4 code for parameter estimation example.

Note : We have introduced the input variable, [u], as a constant state variable of value equal to 1. This is simply a trick to let RK4 implement formulas that will refer to cells in the [u] column. The actual value of [u] will be replaced later by values from raw data.

After opening the file, the [**Initialization**] folder tab should show up. Choose the [**Parameter Estimation**] option. You can then add the file containing the data set using the [**ADD/Browse...**] button as shown in Figure 20.
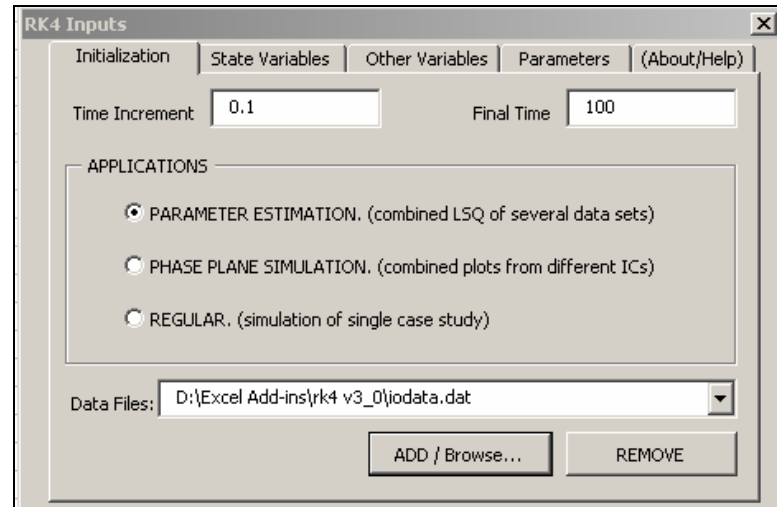
Figure 20.

Then click the [**OK**] button. You will then be prompted to either save the model file or not. Afterwards, the [**Select/Label Data Columns**] window will appear as shown in Figure 21.
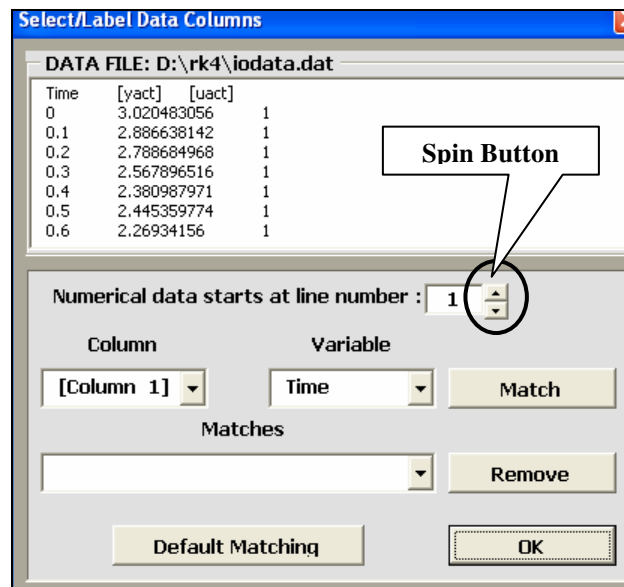
Figure 21. Column-Data matching interface.

(Note: The file containing the data should be a text file where the columns are separated either by spaces or tabs.)

For our example, since the numerical data starts at line 2 (with the first line containing labels of each column as given in the data file) click the spin button up-arrow to change the value from 1 to 2. Next, obtain the matches as shown in Figure 22 and then click the [**OK**] button.
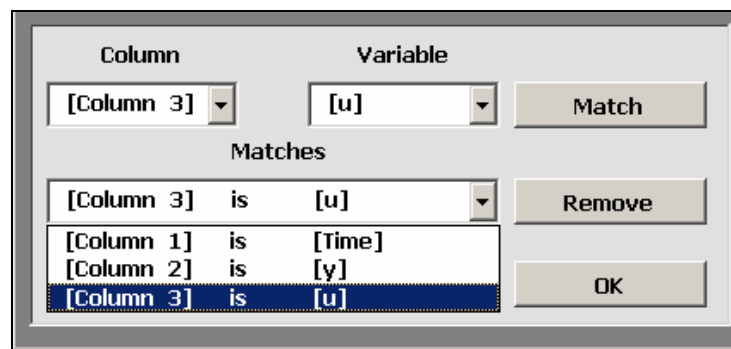
Figure 22. The desired matching for the parameter estimation example.

The spreadsheet as shown in Figure 23 should now result.

Figure 23. The resulting spreadsheet for the parameter estimation example.

In the "Data and Error Analysis" block, "[y]" is from the raw data, "[y]*" is a link to [y] in the "Simulated Results" block and "d[y]^2" is the squared error between [y] and [y]*. This is similarly the case for "[u]", "[u]*" and "d[u]^2".

As we had planned earlier, we want the [u] variable used in the simulation to actually come from the data. To do so, we can copy the [u]-values in the "Data and Error Analysis" block to the [u]-values in the "Simulation Results" block, as shown in Figure 24. (Note: it is recommend to use the [Paste Special]→[Values] option.)

Figure 24. Copying of the u-column in the data block to the u-column in the simulation block.

We are now ready to minimize the root mean squared (RMS) error. The
RMS formula should already be contained in the cell next to the "RMS:"
label. Select this cell and then select the menu item: [**Tools**]→[**Solver**]
and choose the "minimize" button while selecting to change the cells
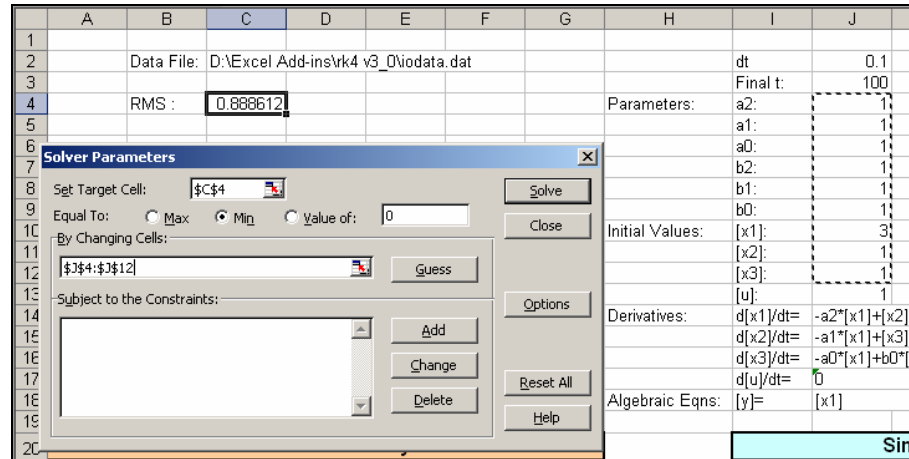shown enclosed by dotted lines in Figure 25. Click [**Solve**].

Figure 25. Using the SOLVER® Add-in to minimize RMS cell.

To see how well the model approximates the data, click on the [**PLOT**]
button in the toolbar. After the plotting interface window appears, select
to plot Time vs. [y] and also click on the "Include data points" option as
shown in Figure 26. Then click on the [**PLOT**] button of the interface
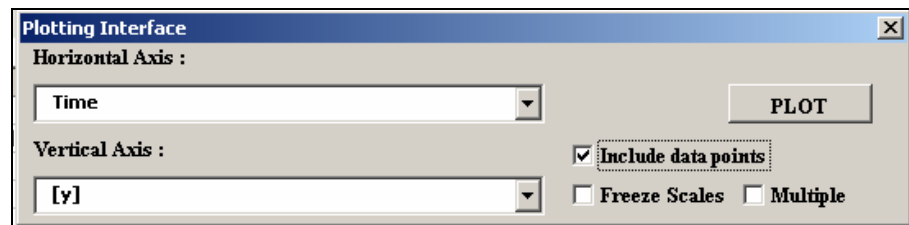window.

Figure 26.

You can also change the location of the plot.   For instance, you can move
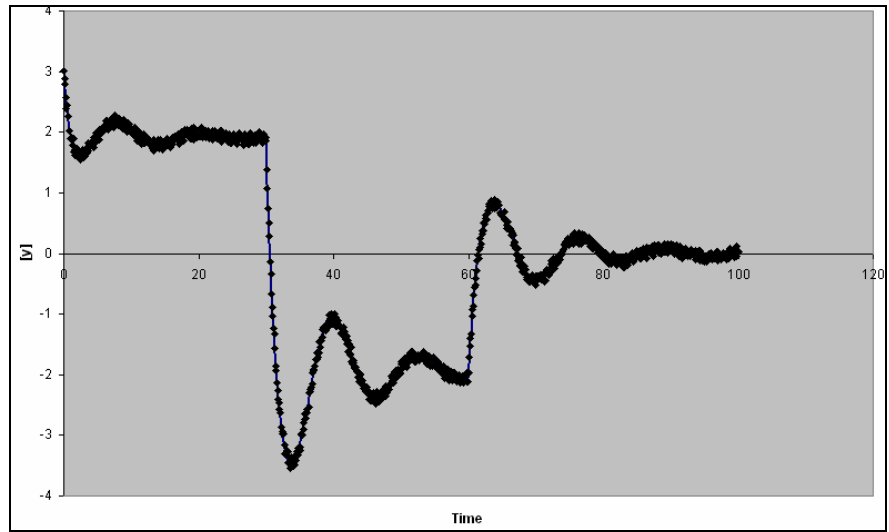it to a separate chart sheet as shown in Figure 27.

Figure 27. A plot of the simulation result together with raw data.

Using Excel routines, the data-series could also be adjusted in order to zoom-in on the results as shown in Figure 28.
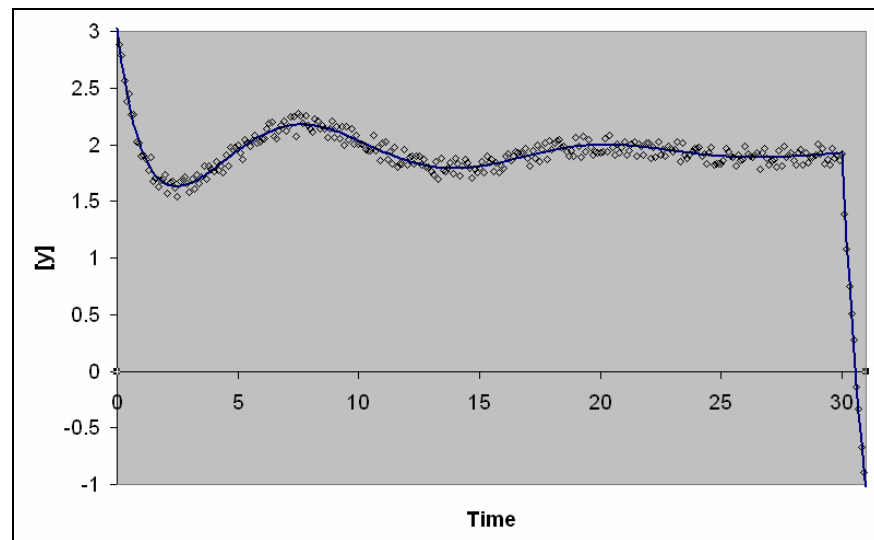

Figure 28. Zoomed portion of Figure 27.

Application IV. Combining different plots in one chart.

Recommended use: when several cases are better compared by combining the plots in one chart, e.g. phase plane portraits.

Example Scenario:

Given the system described by

$$\frac{dx_1}{dt} = a_{11}x_1 + a_{12}x_2$$

$$\frac{dx_2}{dt} = a_{21}x_1 + a_{22}x_2$$

Where,

$$a_{11} = -\frac{4}{3}, \qquad -2 < a_{11} < 2$$

$$a_{12} = \frac{1}{3}$$

$$a_{21} = -\frac{4}{3}$$

$$a_{12} = -\frac{8}{3}$$

And the initial conditions are allowed to be within the following ranges:

$$-10 < x_1(0) < 10$$
$$-10 < x_2(0) < 10$$

Example Session:

Using WORDPAD or NOTEPAD, write (or cut-and-paste) the code shown in Figure 29 to a "*.rk4" file.

```
'
'        Time Settings
'        =============
'
dt: 0.02
tfinal: 5
'
'
'        state equations
'        ===============
'
[x1], Initial Value: -10, Deriv:a11*[x1]+a12*[x2], Min: -10, Max: 10
[x2], Initial Value: -10, Deriv:a21*[x1]+a22*[x2], Min: -10, Max: 10
'
'        parameters
'        ==========
'
a11,    Value: -1.333,    Min: -2,    Max: 2
a12,    Value: 0.333
a21,    Value: -1.333
a22,    Value: -2.667
```

Figure 29. RK4 code for the phase plane example

Open this code with RK4. The [**Initialization**] folder tab window should appear. This time choose the [**Phase Plane Simulation**] option, and some more controls should appear as shown in Figure 30.
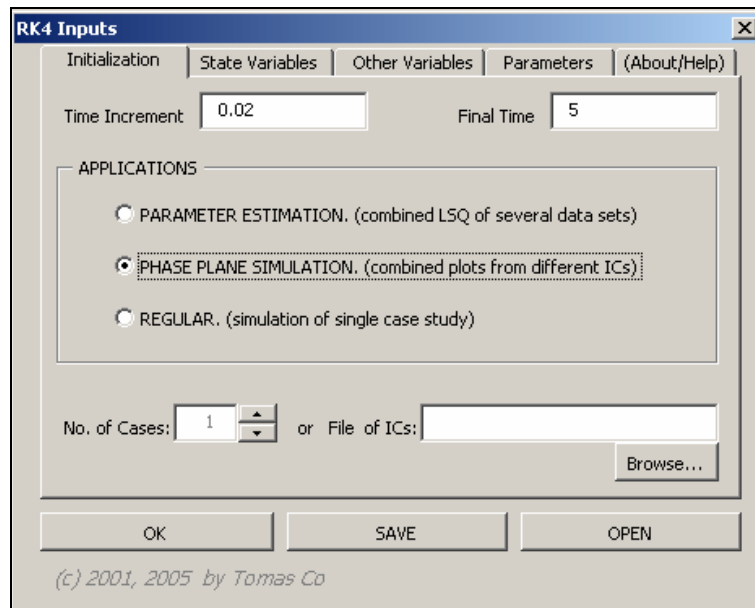

Figure 30.

The "cases" here are meant to indicate different initial conditions. There are two approaches available. The first approach is to choose the number of cases of the phase plane portraits using the spin button. The other is to use the initial conditions from an existing text file. For our example, we

will first choose the spin button approach and click-on the up-arrow until we get 4. Click on the [**OK**] button. The spreadsheet calculations will commence.

Using the scroll bars, change the values of the initial conditions to reproduce the values shown in Figure 31. (Note: that the worksheets in an RK4 workbook will be renamed "main", "Case1", "Case2, etc. These names are used by subroutines in the RK4 add-in so changing these names can result in unpredicted errors.)

Figure 31. Spreadsheet after the values have been changed using the scroll bars.

Next, click on the [**PLOT**] button in the toolbar to obtain the "Plotting Interface" window. Check-on the [**Mulitple**] option. The [**Plot**] button should have changed to [**mPlot**]. Also, other control objects should appear as shown in Figure 32. Select [x1_Case1] and [x2_Case1] as the entries in the "Horizontal Axis" and "Vertical Axis", respectively. We can use the [**ADD**] and [**DELETE**] buttons to manually choose among the variables across different cases that we want to plot. However, as a shortcut for the phase-plane plot, choose the [**ADD ALL CASES**] button.
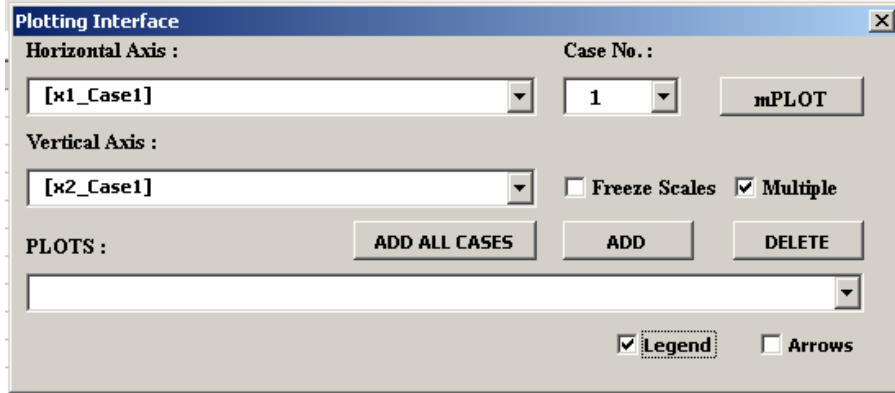
Figure 32. Plotting interface for the phase plane example.

Since this will be a multiple plot, it is recommended to check-on the [**Legend**] box. Next, click on the [**mPlot**] button. A plot showing the four trajectories should now appear as shown in Figure 33.
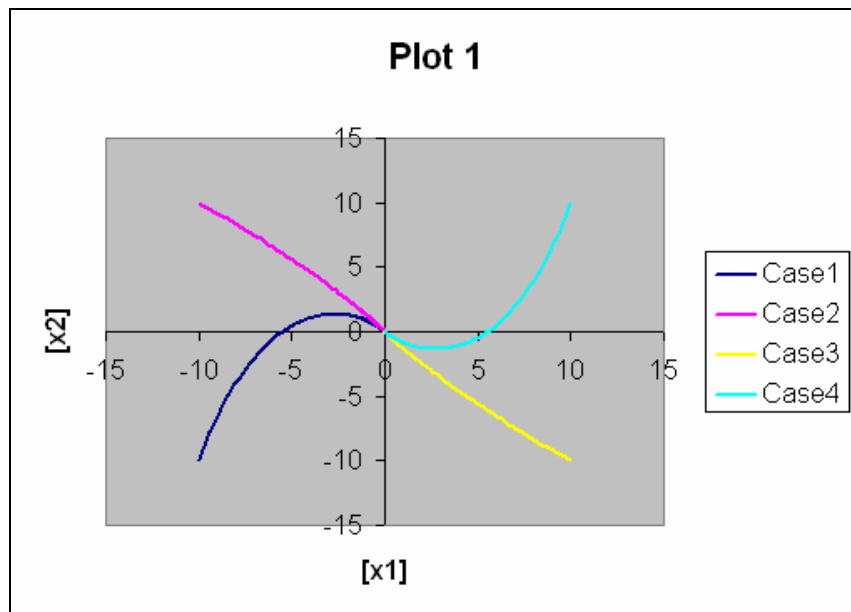

Figure 33. A multiple plot of the phase plane with [**Legend**] selected.

Usually, we may want a companion plot that shows the arrows of the trajectories. To do so, proceed as before except that you check-on the [**Arrows**] box instead. (Note: the [**Arrows**] and [**Legend**] options are mutually exclusive choices.) The plot with arrows should now appear as shown in Figure 34.
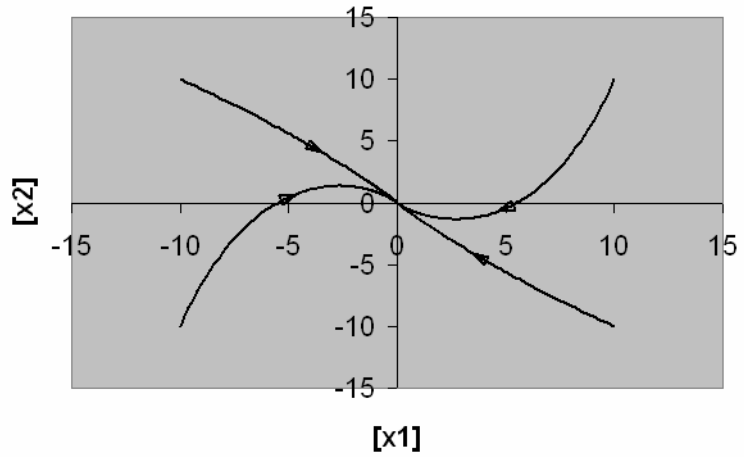
Plot 2

Figure 34. A multiple plot of the phase plane with [**Arrows**] selected.

To explore how the phase portrait changes according to changes in the value of parameter a_{11}, move the scroll bar attached to this parameter. One should be able to observe how the phase portrait changes from an improper node to a stable node and then to a saddle. Of course, the initial conditions may need to be moved around to improve the image. For instance, the various scroll bars can be adjusted to show the saddle given in Figure 35.
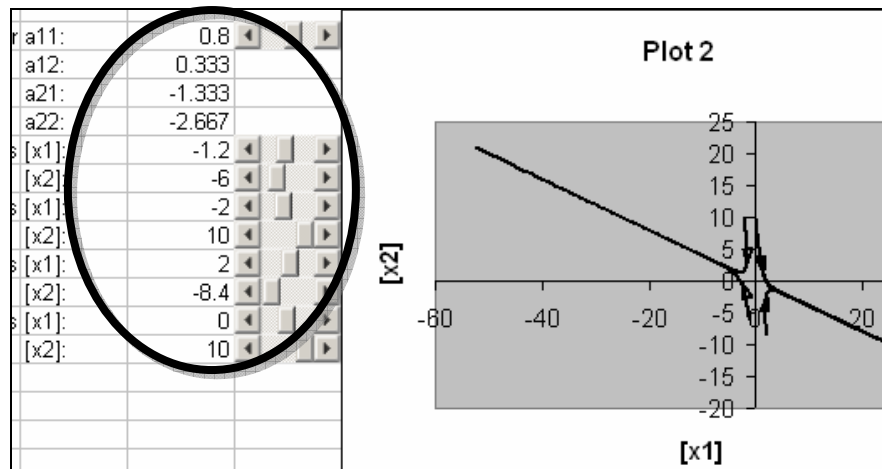

Figure 35. By varying initial conditions and parameter, changes in the phase plane can be observed.

To continue our example, let us suppose that we want the initial conditions to be a set of uniformly separated points at a circle centered around the origin.

First, open a new workbook. (Note: It is recommended that additional calculations be done on a new workbook rather than a new worksheet) An example spreadsheet is shown in Figure 36.

	A	B	C	D	E	F
1						
2		radius	1			
3		pi	3.14159			
4						
5		theta	x	y		
6	1	0	1	0		
7	2	0.314159	0.951057	0.309016742		
8	3	0.628318	0.809017	0.587784823		
9	4	0.942477	0.587786	0.809016526		
10	5	1.256636	0.309018	0.951056188		
11	6	1.570795	1.33E-06	1		
12	7	1.884954	-0.30902	0.95105	=$C$2*SIN(B16)	
13	8	2.199113	-0.58778	0.80901		
14	9	2.5137	-0.80902	0.587786		
15	10	2.827	-0.95106	0.30901		
16	=$C$3/10*(A13-1)		-1	2.65359E-06		
17	12	3.455749	-0.95106	-0.309014218		
18	13	3.769908	-0.80902	-0.587782676		
19	14	4.084067	-0.5877	=$C$2*COS(B23)		
20	15	4.398226	-0.3090			
21	16	4.712385	-4E-06	-1		
22	17	5.026544	0.30901	-0.951057828		
23	18	5.340703	0.58782	-0.809019646		
24	19	5.654862	0.809014	-0.587789117		
25	20	5.969021	0.951055	-0.309021789		
26						

Figure 36. Calculations of the initial conditions at a circle centered at the origin.

Copy the block that as shaded in Figure 36 and paste to a WORDPAD or NOTEPAD using [**Paste Special...**]➔[**Unformatted Text**] as shown in Figure 37.
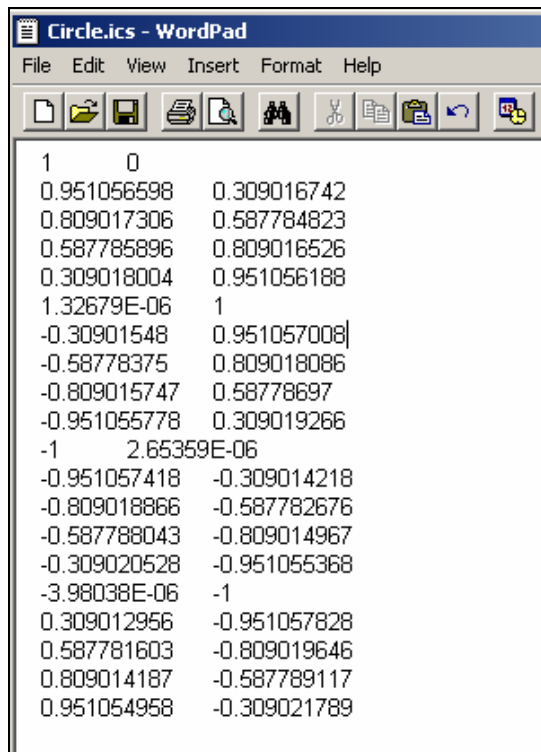

Figure 37. A WORDPAD file containing the resulting calculations of the initial conditions.

It is recommended to save the text file with the extension of "*.ics". For our example, suppose we had saved the file as "Circle.ics".

Next open another new workbook. When we left the other workbook, the toolbar still says "PLOT". When the worksheets are named "Sheet1", etc., clicking on the "PLOT" button will toggle it back to the "RK4" button as shown in Figure 38.
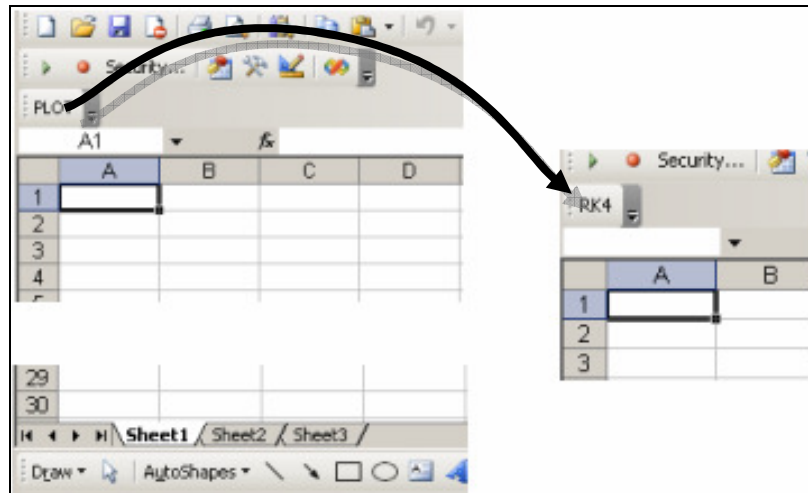
Figure 38.

Follow the same procedure as before, except that we can use the approach of loading the initial conditions from the IC file as shown in Figure 39.
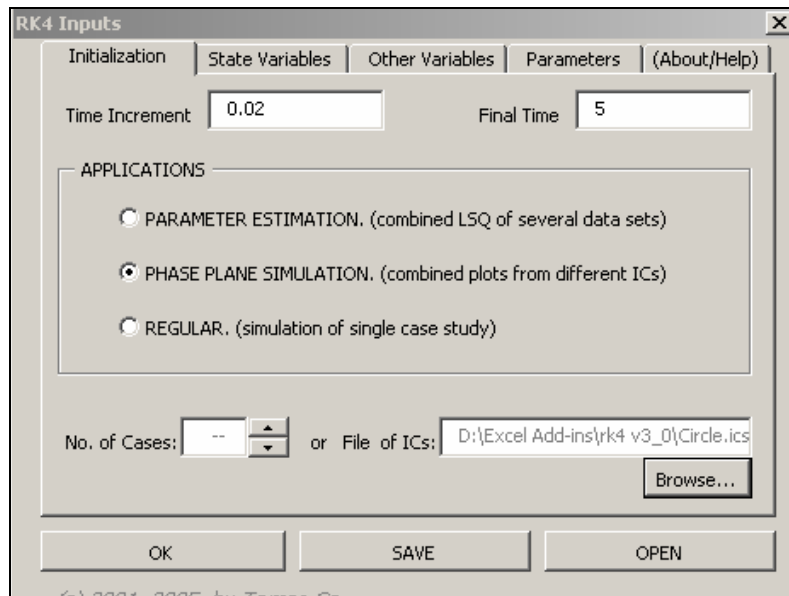

Figure 39.

After clicking [**OK**], the spreadsheet should show the 20 pairs of initial conditions for each case. After choosing to [**mPlot**] all the different cases, the plot will show up at the bottom of the 20th case. This mean we need to scroll the spreadsheet down to see the plot. We can resize the plot as shown in Figure 40.
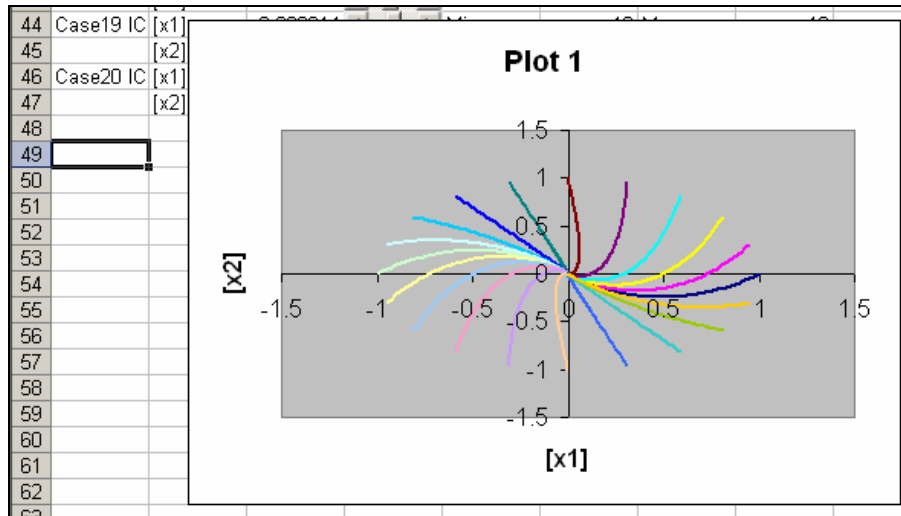
Figure 40.

Application V. Parameter estimation from combining different data.

Recommended use: Laboratory data sets obtained with non-uniform sampling time instants.

Example Scenario:

Using data from two different data sets (case1.dat and case2.dat), we want to fit the following model:

$$\frac{dx_1}{dt} = -(k_{21} + k_{31})x_1 + k_{12}x_2 + k_{13}x_3$$

$$\frac{dx_2}{dt} = k_{21}x_1 - (k_{12} + k_{32})x_2 + k_{23}x_3$$

$$x_3 = 1 - (x_1 + x_2)$$

Example Session:

Using WORDPAD or NOTEPAD, write (or cut-and-paste) the code shown in Figure 41.

```
'
'      Sampling interval and final time
'      --------------------------------
'
       dt: 0.02
       tfinal: 5
'
'      Differential Equations
'      ----------------------
'
       [x1], Initial Value: 1, Deriv: -(k21+k31)*[x1]+k12*[x2]+k13*[x3]
       [x2], Initial Value: 0, Deriv: k21*[x1]-(k12+k32)*[x2]+k23*[x3]
'
'      Algebraic Equations
'      -------------------
'
       [x3], Eqn: 1-[x1]-[x2]
'
'      Parameters
'      ----------
'
       k21,    Value: 1
       k31,    Value: 1
       k12,    Value: 1
       k32,    Value: 1
       k13,    Value: 1
       k23,    Value: 1
```

Figure 41.

Opening the code, go to the [**Initialization**] folder tab. Choose the
[**Parameter Estimation**] selection and using [**ADD/Browse...**] button,
choose to load the two data files as shown in Figure 42. Click [**OK**].
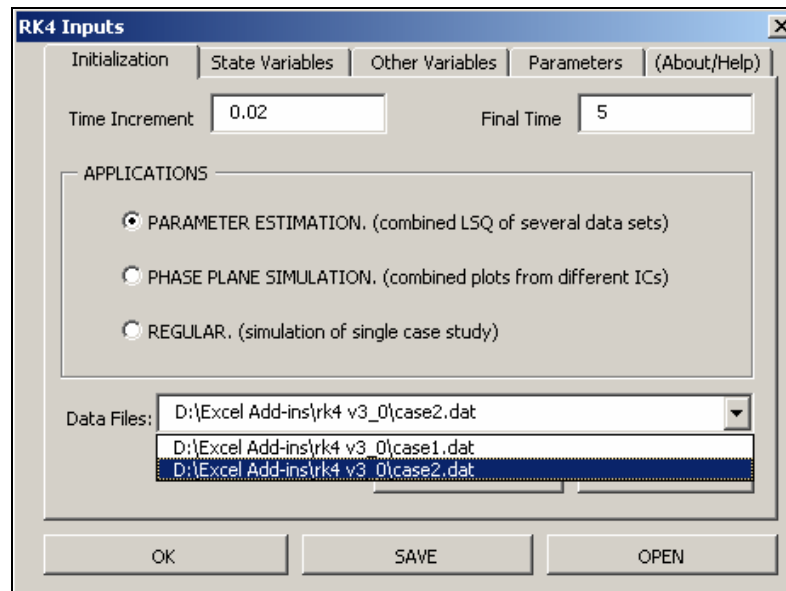

Figure 42.

Choose to save model file or not. The next window will be to match the
columns to the variables. From Figure 43, since the data given in
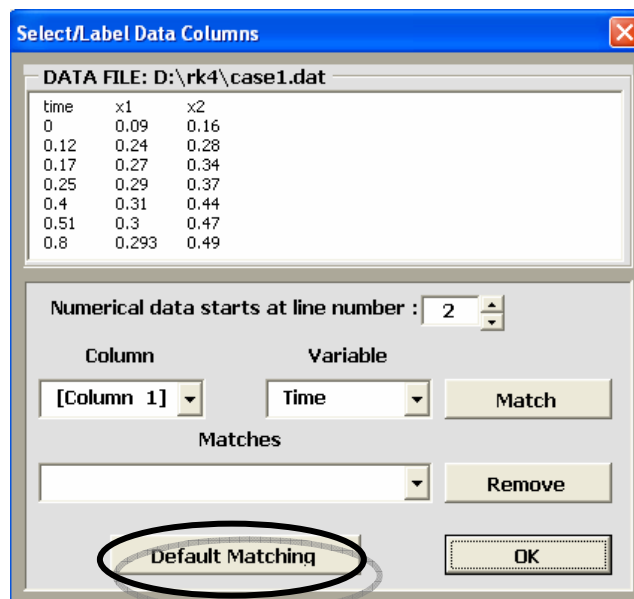Case1.dat has the same sequence of variables keyed in from the model, we
could use the short-cut [**Default Matching**] button.

Figure 43.
Then click [**OK**]. Another short-cut option "Auto-Match" will appear.

This will only show up after the first data set. Choosing [**Yes**] would mean that all the data-sets have the same column matches. Choosing [**No**] would show another matching window similar to that shown in Figure 43 above.
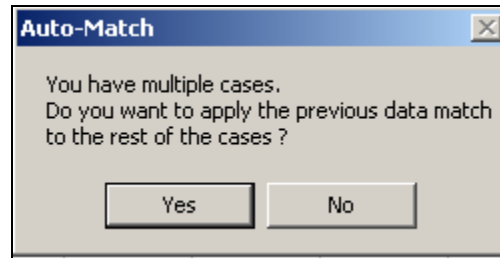

Figure 44.

Choose [**Yes**]. The spreadsheets should now result. The [**main**] worksheet contains the parameters and initial conditions. It also includes the cell for the RMS calculation which involves the squared errors in both spreadsheets named Case1 and Case2.

Next, select from menu, the item: [**Tools**]→[**Solver**]. Choose the "minimize" option and then select to change the cells shown enclosed as dotted lines in Figure 45. Then click [**Solve**].
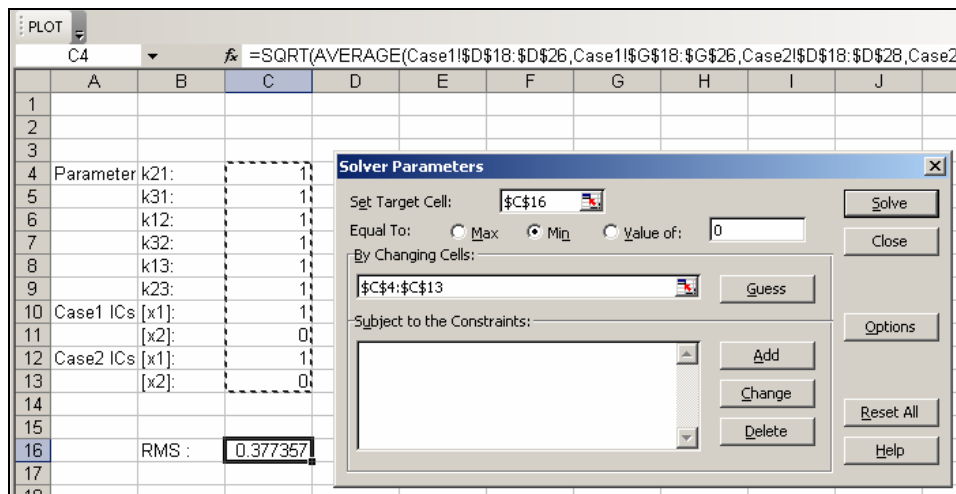

Figure 45.

Click on [**Plot**] and then modify the "Plotting Interface" window to match the one shown in Figure 46 (select the [**include data**] option as well as use the [**ADD**] button). Then click [**OK**] to obtain the time-plots shown in Figure 47. We can also use the [**Plot**] toolbar to show a similar time-plot for case 2 and the phase plane as shown in Figures 47 and 48, respectively.
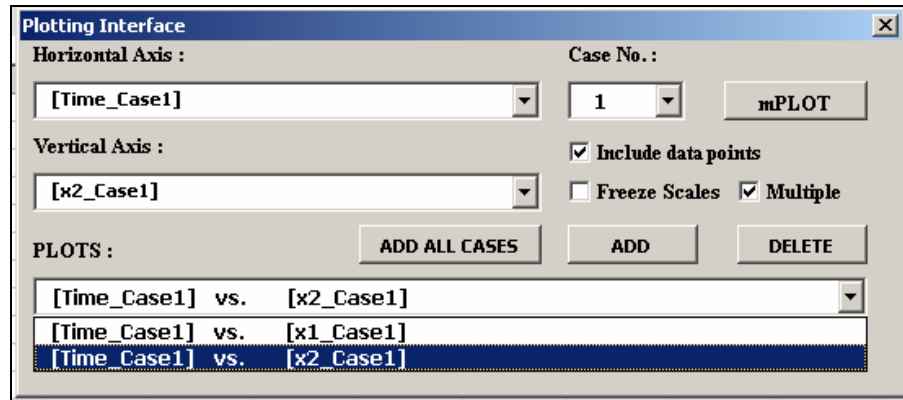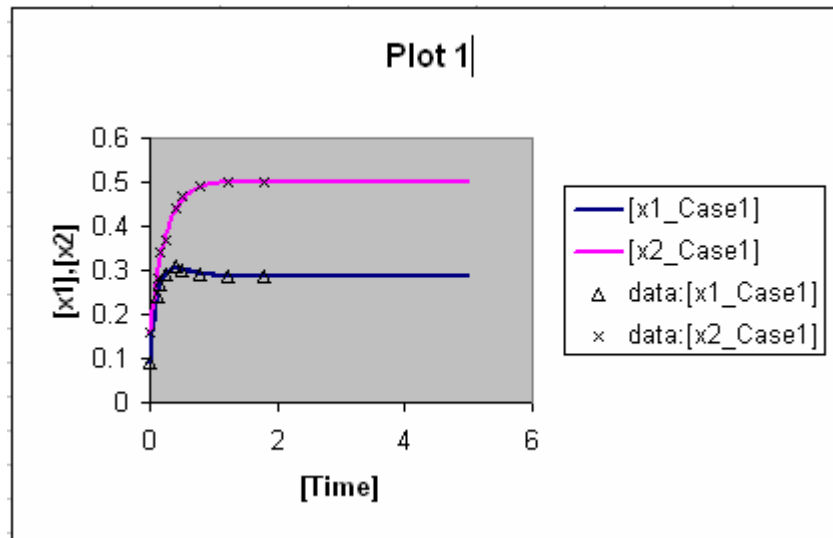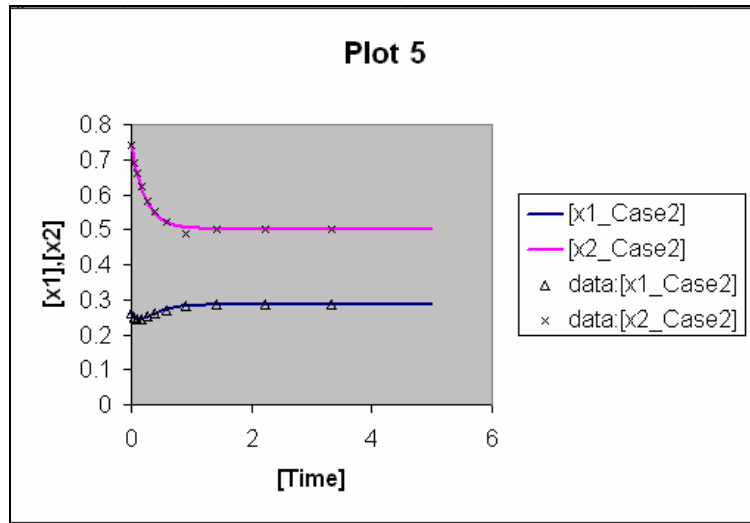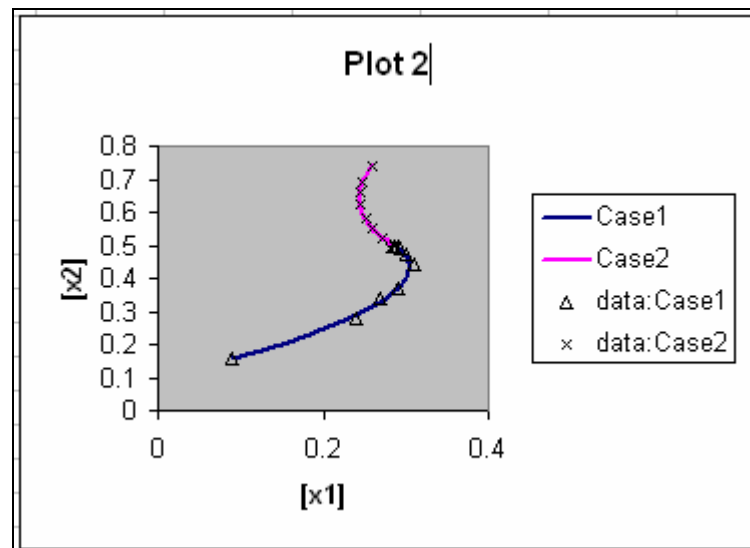

Figure 45.

Figure 46.

Figure 47.

Figure 48.