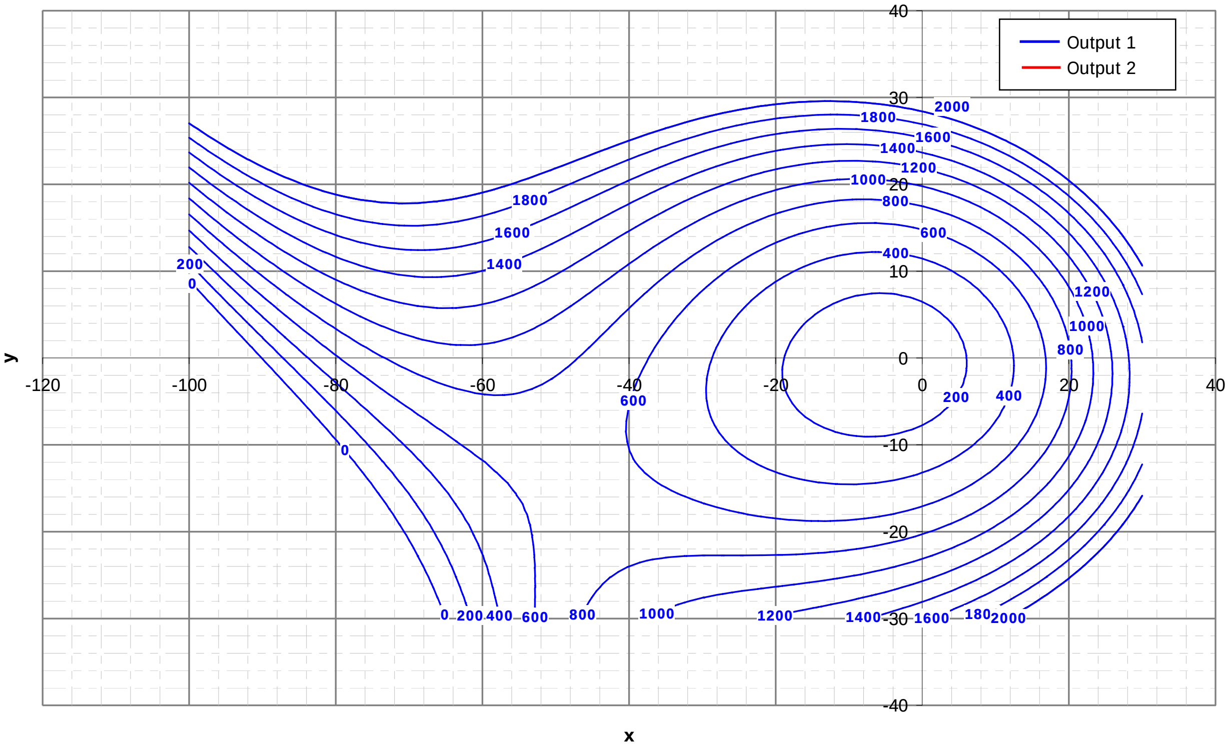
# Numerical Analysis Notes

Foxes Team

## Plotting of z = f(x,y) contour-lines with Excel

### Macro isol.xls

The Excel (XP/2003) macro **isol.xls**, developed by **SimonLuca Santoro** and kindly released in the free public domain, allows to plot iso-levels, or contour lines, of a bi-variate explicit function f(x,y). The output, of good and accurate quality, are not simply static bitmap but there are true Excel graphs that can be manipulated with the standard Excel tools.
The following picture is an example of the macro output

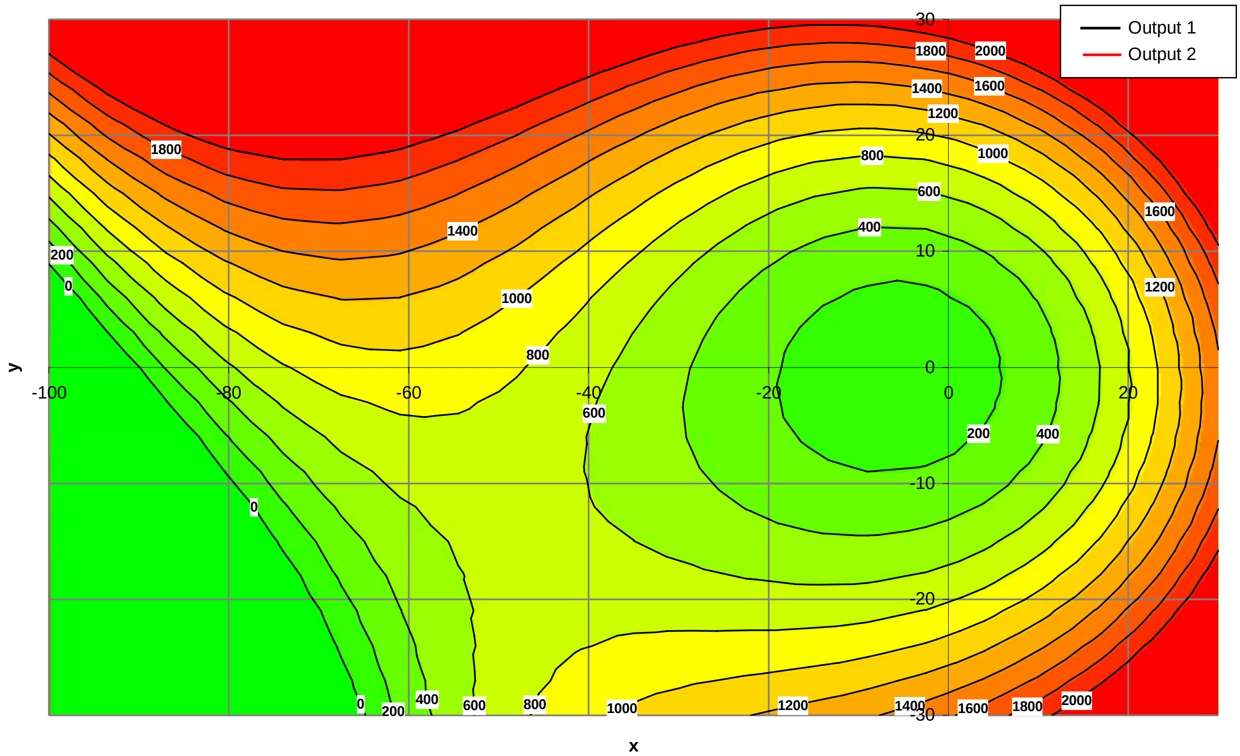



The version 2 of this macro can output colored maps thanks to the **Mapper** macro developed by **Robert de Levie** for his MacroBundle collection.

http://www.bowdoin.edu/~rdelevie/excellaneous/

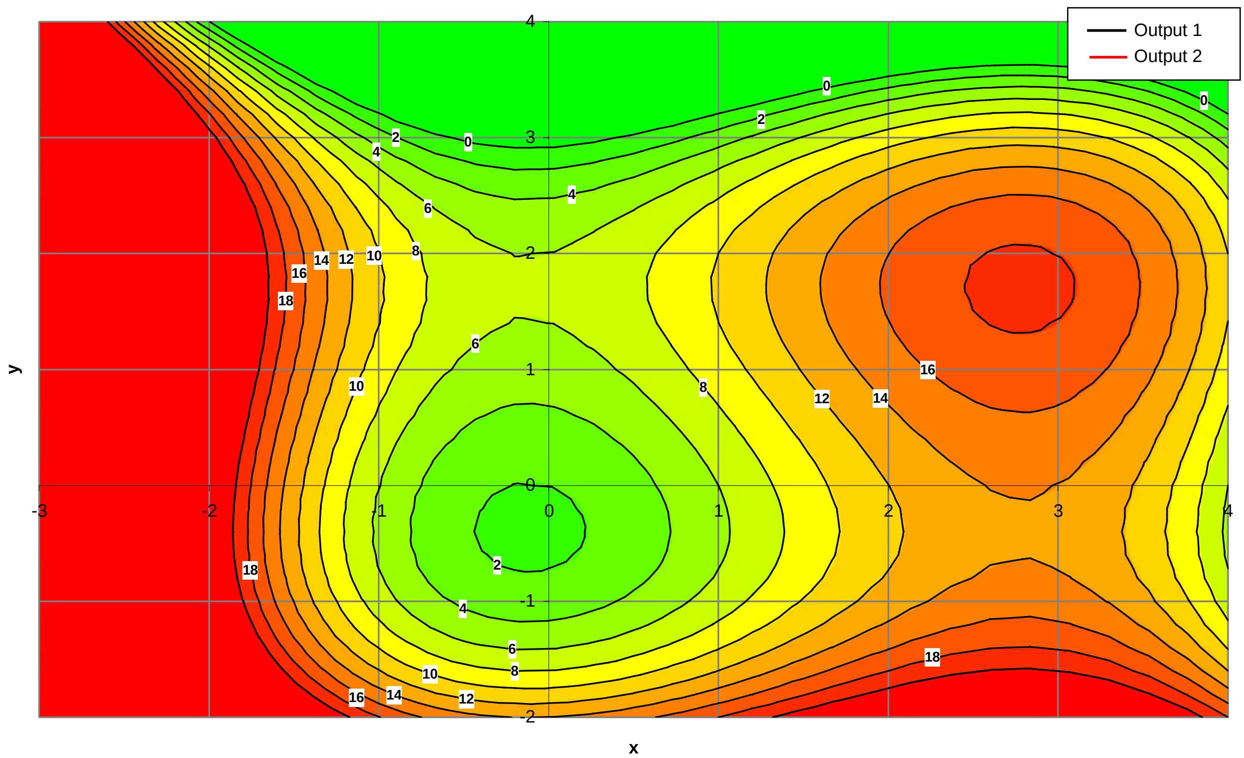
A detailed explanation of this macro can be found in the book "*Advanced Excel for scientific data analysis*", of the same author.

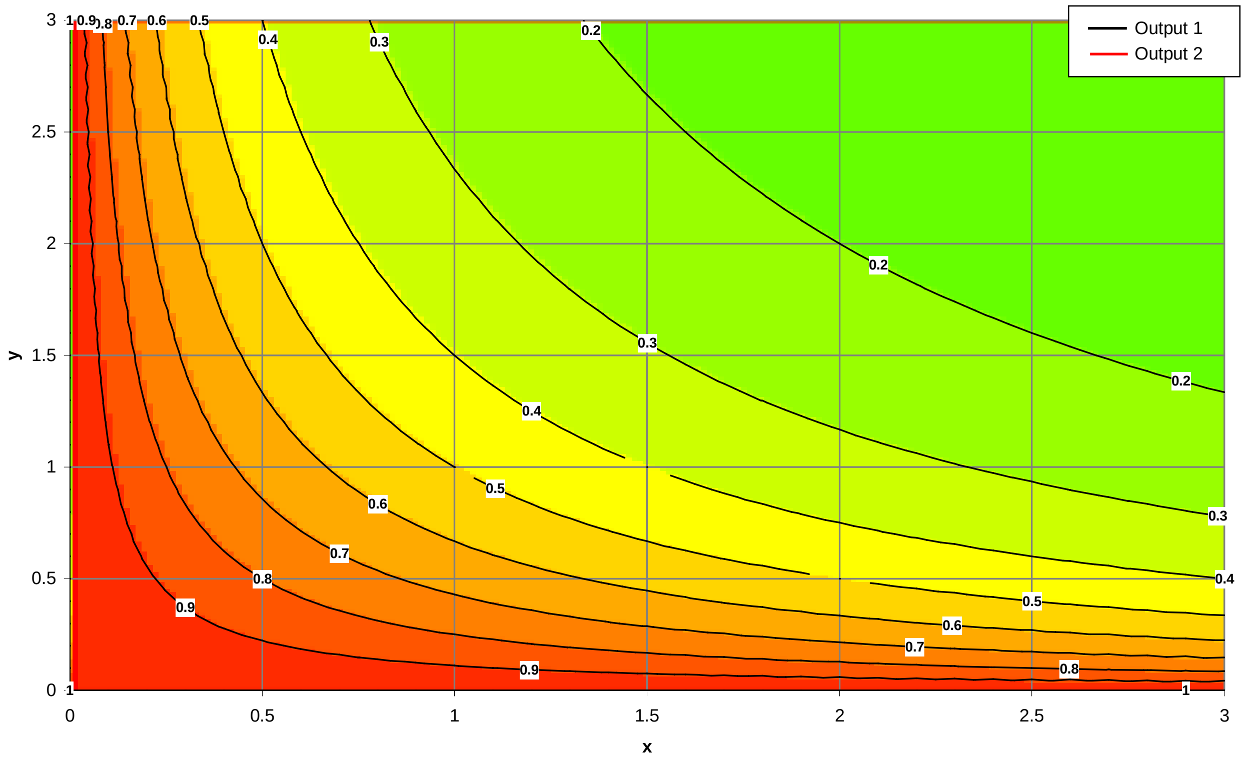
Generating colored maps together with contours lines, allows us to get very interesting and beautiful graphs.




As we can see, the colors enhance the global 3D effect while, at the same time, the iso-lines assure the needed precision for scientific computing

Other examples are the following






The macro **isol.xls** outputs the graphs in separated files xls, that are, generally, quite big (1 - 1.5 MB). Successively they can be re-opened an manipulated without the macro isol.xls.
Note. The zip file also contains the template isol_output_t.xls. Do not write this file. It must be only copied in the same directory of the isol.xls macro

The macro creates graphs in three different ways:

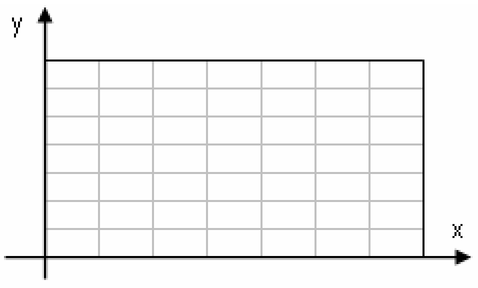
- by rational function of $4^{-th}$ degree P(x,y)/Q(x,y)
- by data table [xi, yi, zi]
- by Excel formula

**Algorithm**
The algorithm for iso-level plotting bases itself on the triangolarization of the rectangular domain $D \equiv \{ x, y : x_{min} \le x \le x_{max} , y_{min} \le y \le y_{max} \}$

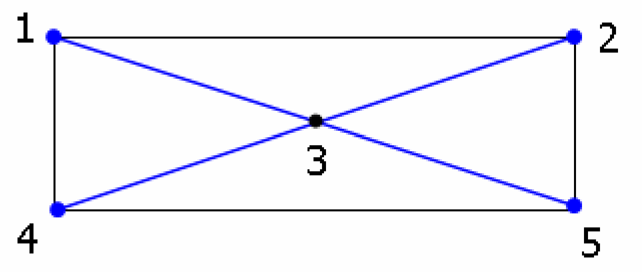
Synthetically, the basic steps are:

1. Partitioning in rectangular sub-domains
2. Partitioning of each sub-domain in 4 triangles
3. Evaluation of z=f(x,y) at the vertices ($P_1$', $P_2$', $P_3$') of each triangle.
4. Identification of the interpolation plane for the vertices of each triangle
5. Identification of the segment AB, intersection of the triangle and the plane $\pi$, $z = z_i$

<u>1) Partitioning in rectangular sub-domains</u>




2) Partitioning of each sub-domain in 4 triangles




3) Evaluation of $z = f(x,y)$, at the vertices of each triangle: T123, T235, T134, T345

4. Identification of the interpolation plane for the vertices of each triangle

For simplicity we refer to the triangle T123
Taking:

$z_1 = f(x_1,y_1)$, $z_2 = f(x_2,y_2)$, $z_3 = f(x_3,y_3)$

We define the interpolating plane

$p(x,y) = a+b\,x+c\,y$

The coefficients a, b, c are determined by the following formulas

$a = [(y_3\,x_2 - x_3\,y_2)\,z_1 + (y_1\,x_3 - x_1\,y_3)\,z_2 + (y_2\,x_1 - x_2\,y_1)\,z_3\,]\,/\,d$
$b = [(y_2 - y_3)\,z_1 + (y_3 - y_1)\,z_2 + (y_1 - y_2)\,z_3\,]\,/\,d$
$c = [(x_3 - x_2)\,z_1 + (x_1 - x_3)\,z_2 + (x_2 - x_1)\,z_3\,]\,/\,d$

where: $d = x_1\,y_2 + y_1\,x_3 + y_3\,x_2 - y_1\,x_2 - x_3\,y_2 - x_1\,y_3$

The more the domain is small, the more the plane approximates the surface.

5) Identification of the segment AB

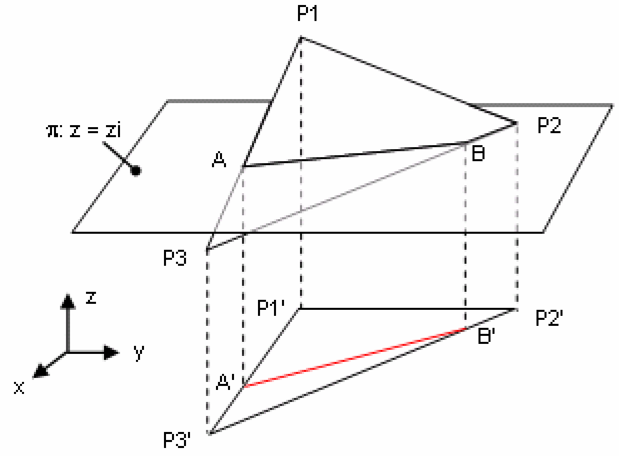
At this step, we find the segment AB, intersection between the interpolation plane p(x,y) and the horizontal plane z = zi, where zi is the quote of the iso-level that we want to trace. The projection of the segment AB on the plane xy gives us the new segment A'B'
For each side of the triangle, determined by the points $P_1(x_1, y_1, z_1)$, $P_2(x_2, y_2, z_2)$ , the correspondent projection point P'(x,y) is given by the formulas:

$x = [(a - z_i)(x_1 - x_2) + c\,(x_1 y_2 - x_2 y_1)] / m$
$y = [(a - z_i)(y_1 - y_2) + b\,(x_2 y_1 - x_1 y_2)] / m$

where: $m = b\,(x_2 - x_1) + c\,(y_2 - y_1)$

This operation must be repeated for each side of the triangle simply by indices permutation.
Second side: $x_2 \rightarrow x_3$ ; $x_1 \rightarrow x_2$ ; $y_2 \rightarrow y_3$ ; $y_1 \rightarrow y_2$
Third side: $x_3 \rightarrow x_1$ ; $x_2 \rightarrow x_3$ ; $y_3 \rightarrow y_1$ ; $y_2 \rightarrow y_3$

At the end, for each triangle, we have 2 points, A' B', on the plane z = 0, belong to the projection of the segment AB.
The trace A' B', image of AB on the plane xy, approximates a little piece of the iso-level for $z = z_i$. The approximation increases when the area of the sub-domains becomes small.




The advantage of this free-gradient method is its robustness because it can also work with irregular, non differentiable, surfaces. The drawback is an high computational effort (about 100 operations for triangle) that produces a quite long elaboration time (minutes)

Parametric Formulas. In order to reduce the computation time we can adopt a variant that avoids the explicit calculus of the interpolation plane by using the parametric formulas of the triangle segments $P_1(x_1,y_1,z_1)$, $P_2(x_2,y_2,z_2)$, $P_3(x_3,y_3,z_3)$
The coordinates of the image points A', B', C' , if exist, are given by the following simpler formulas:

$$A' = \begin{cases} x_1 + t_1(x_2 - x_1) \\ y_1 + t_1(y_2 - y_1) \end{cases} \quad , \quad t_1 = \frac{z_i - z_1}{z_2 - z_1} \quad , \quad z_2 \neq z_1$$

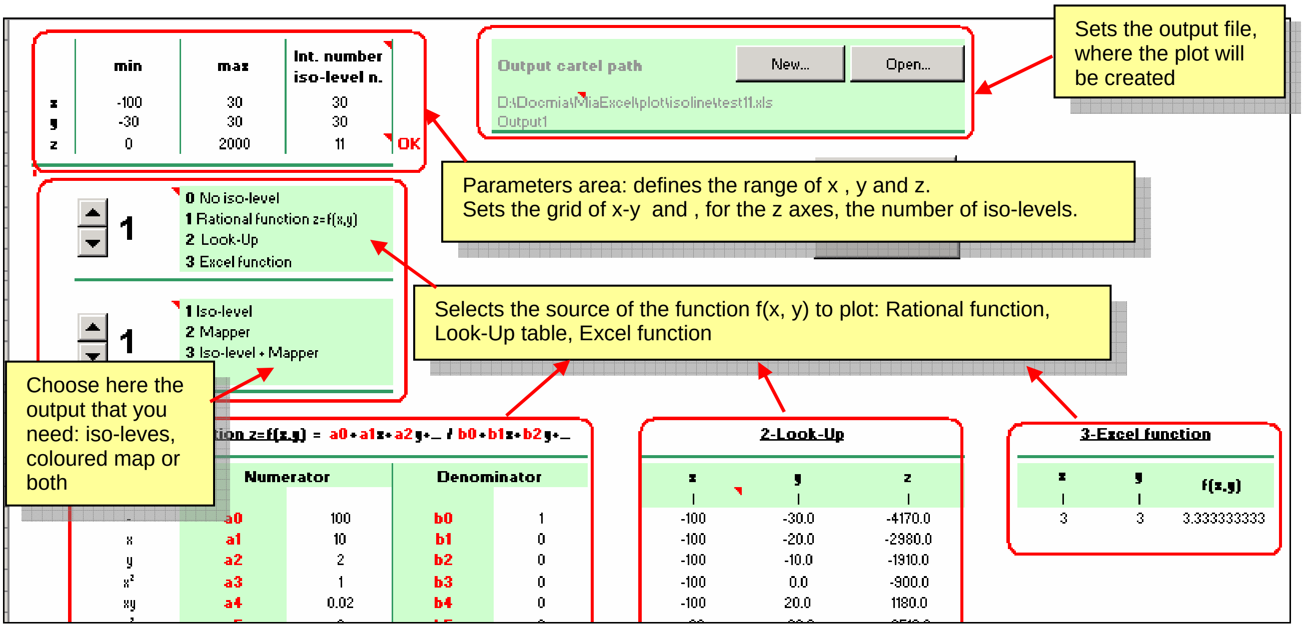
$$B' = \begin{cases} x_1 + t_1(x_3 - x_1) \\ y_1 + t_1(y_3 - y_1) \end{cases} \quad , \quad t_1 = \frac{z_i - z_1}{z_3 - z_1} \quad , \quad z_3 \neq z_1$$

$$C' = \begin{cases} x_2 + t_1(x_3 - x_2) \\ y_2 + t_1(y_3 - y_2) \end{cases} \quad , \quad t_1 = \frac{z_i - z_2}{z_3 - z_3} \quad , \quad z_3 \neq z_2$$

We pay attention to choose only the points where is $0 \leq t_i \leq 1$
Generally, this variant reduces of about 1/3 the total elaboration time-

## How to use the macro isol.xls

First of all, extract the files isol.xls and isol_output_t.xls from the pack isol.zip and put them in the same directory that you like.
Now start Excel and open the file isol.xls (it contains macros, so remember to activate the macro)
In the sheet "input1", the controls are grouped in several areas




The first thing to do is the choice of the output file. Click on "new…" button to open the dialog, insert the name that you want (example myplot1.xls) and give OK.
From now on, all the output will be redirect to this file until you will change it.
Now we have to choose the function source. This depends by the type of problem that we have. Assume, for example, that we have to plot the contours of a rational function such as:

$$f(x,y) = \frac{x\,y}{2\,x\,y^2 + 1}$$

for $0 < x < 2$ and $0 < y < 8$, and we want to plot 10 iso-lines spaced by 0.1 from 0 to 1
For the beginning, we chose a grid of 40 x 40 nodes.

The grid parameters influence the global accuracy of the plot and, of course, the total elaboration time. If the plot will not look sufficiently accurate we should increase the grid. Remember only that the time increases sharply with the grid. (For example, if the time required for a 40x40 grid is 10 sec, then the time for a 80x80 grid will be 40 sec)

Note. In the plotting domain, the function f(x,y) must be always defined. If a singularity or a computation error raises, the macro stops itself.

Because our function is expressed as a ratio of two polynomials, we can select the “rational” source

1

**0** No iso-level
**1** Rational function z=f(x,y)
**2** Look-Up
**3** Excel function

and input the coefficients:
$a_4 = 1$, $b_0 = 1$, $b_7 = 2$

1-Rational function z=f(x,y) = a0+a1x+a2y+… / b0+b1x+b2y+…

| | Numerator | | Denominator | |
|---|---|---|---|---|
| - | a0 | 0 | b0 | 1 |
| x | a1 | 0 | b1 | 0 |
| y | a2 | 0 | b2 | 0 |
| $x^2$ | a3 | 0 | b3 | 0 |
| xy | a4 | 1 | b4 | 0 |
| $y^2$ | a5 | 0 | b5 | 0 |
| $x^3$ | a6 | 0 | b6 | 0 |
| $x^2y$ | a7 | 0 | b7 | 2 |
| $xy^2$ | a8 | 0 | b8 | 0 |

Select the output “iso-line”

1

**1** Iso-level
**2** Mapper
**3** Iso-level + Mapper

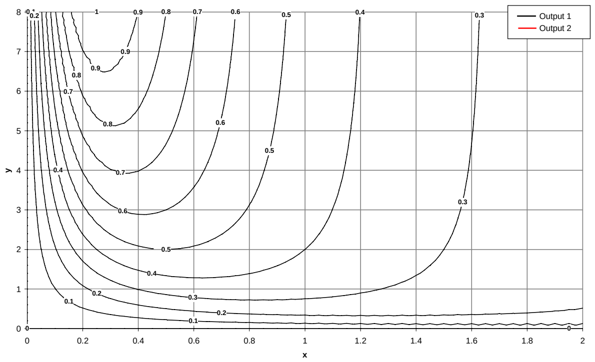
**Tip.** Generally, iso-lines are faster then colored map, so, at the first time, is always convenient select the option 1. Successively, after the plot is adjusted, we can switch to the other options: 2, or 3

The range and grid parameters will look like the following. Remember only to take 11 isol-levels in order to have a step of 0.1, because it is calculated as:

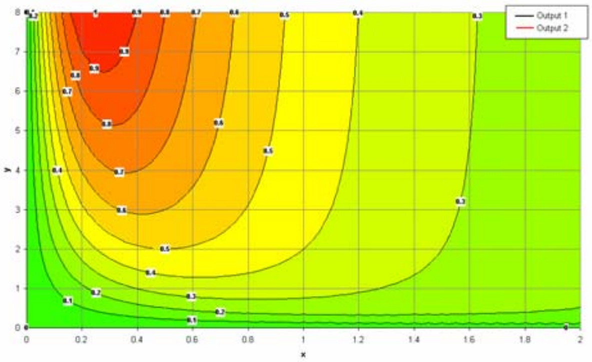
$\Delta z = (x_{max} - z_{min}) / ( n -1)$

| | min | max | Int. number iso-level n. |
|---|---|---|---|
| x | 0 | 2 | 40 |
| y | 0 | 8 | 40 |
| z | 0 | 1 | 11 |

Now, press “Run” to generate the plot




option 1 “Iso-levels”




option 3 “Iso-level+mapper”

We can also define the function f(x, y) by the standard Excel worksheet function Example. Assume that we want to trace the Van der Waals curves using the following normalized equation

$$(p + 3/v^2)(3v - 1) = 8t$$

where *p = P/Pc*, *v=V/Vc*, *t=T/Tc* are the normalize variables
As known, these curves are usually plotted in the plane *p-v* (Clyperon plane). Therefore we assume x ≡ *p* and y ≡ *v*, obtaining

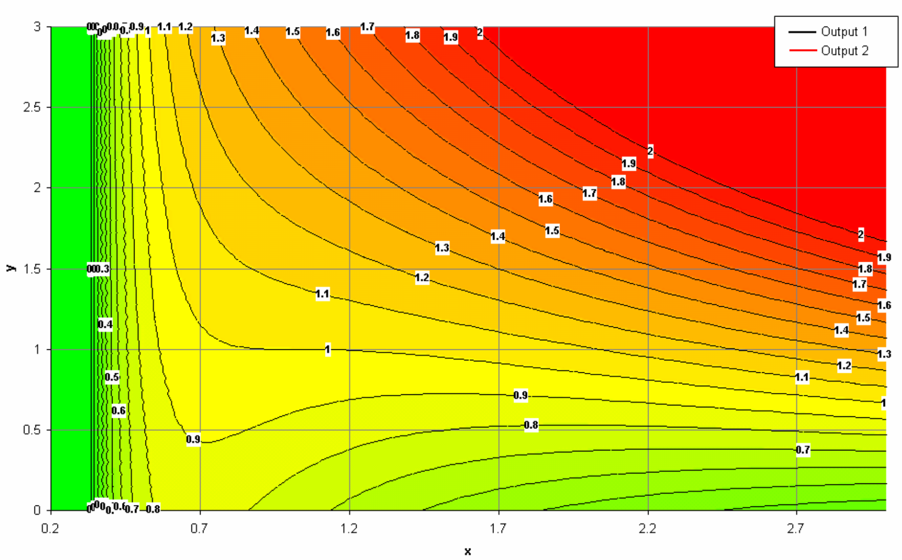
$$t(x, y) = (3/x^2 + y)(3x - 1)/8$$

Also In this case we could transform this expression in rational form, but it is better to insert it directly as an Excel function =(3/M24^2+N24)*(3*M24-1)/8 in “O24” cell

Now insert the range an grid parameters as the following.
Note that we cannot set $x_{min}$= 0 because the function is not defined along the x axes.

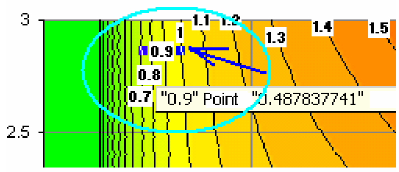
| | min | max | Int. number iso-level n. |
|---|---|---|---|
| x | 0.2 | 3 | 40 |
| y | 0 | 3 | 40 |
| z | 0 | 2 | 21 |

Now, select the option 3 “iso-level + mapper” and press “Run”.



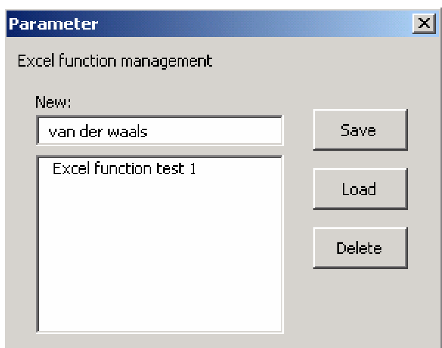

We have previous said that the plot generated are true graph that can be manipulated, if we need, as any other Excel graph. For example, in the previous graph, we note that the labels of the iso-levels between 0 and 0.6 look quite confused because they are too close each other. It would be better eliminate them from the graph. Instead of re-creating the graph we go to the worksheet “output1” and select the range “D1:P1” of the first row containing the values from 0, to 0.6. Deleting these values we will remove the correspondent labels from the plot.

It is also possible re-arrange the labels that are not well disposed by the macro
It can be done simply selecting the label and moving it with the mouse.




**Saving parameter setting**

The current formula and parameters setting can be saved by the “Parameter” button.
Insert an identification string as we like, example “*van der waals*”, and click “Save”.
This parameter setting can be successively recalled simply by the “Load” button
There are 3 different separated lists for Rational. Look-up, and Excel function.



**Data table**

Sometime the function is only known by a tabulated dataset [xi, yi, zi]. In that case comes useful the 2nd option "Look-Up".

The dataset has only this constraint: each abscissa xi must have 2 points at least.

Insert the dataset [xi, yi, zi] in the columns "i", "j", "k" rispectively, starting from the row 24

Then, select the option 2 and start the macro as usual.

Note that "look-up" is much slower then the other methods