

1.1.1 Modifying the Center of an Existing Lattice

The example of Section *Error! Reference source not found.* assumed the (0,0,0) lattice element was at the origin which simplifies the input file. There are many instances where that is not possible. A very common occurrence is when there are an even number of lattice elements as shown below.

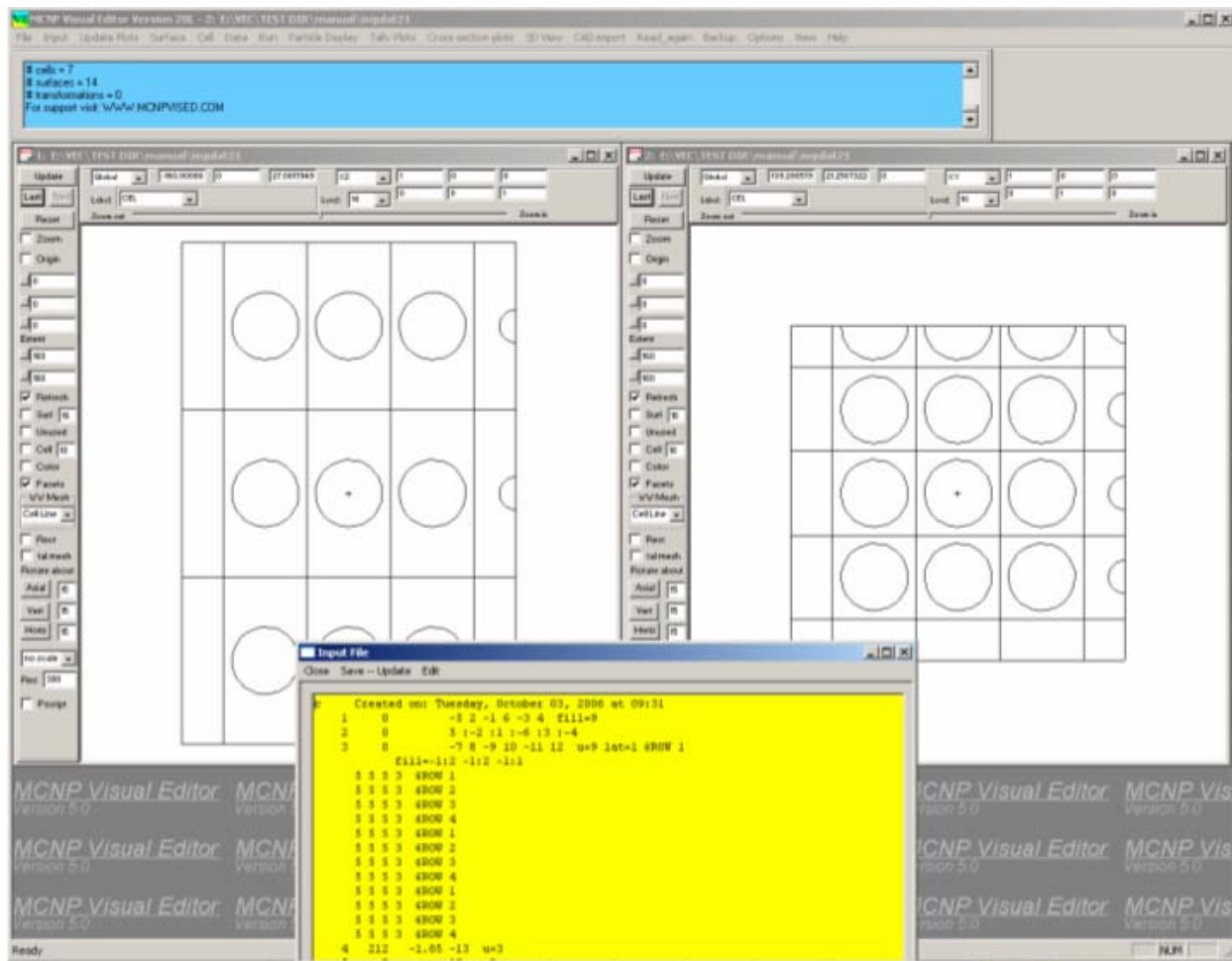


Figure Error! No text of specified style in document.-1 Lattice with an even number of Elements

Figure Error! No text of specified style in document.-1 shows a rectangular lattice with four elements in x and y and three elements in z. Because there is an odd number of elements, the lattice is not centered inside the bounding box. To be centered, the center of the (0,0,0) element must be moved to the top right corner.

Start the Visual Editor.

Click on **File...Open...** and select the **isqulat21** input file.

On the Main Menu, **Click on Update Plots.**

On both plot windows, **change both extents to 160.**

On the main menu, **Click Input** to display the input file.

This input file is identical to the input file used in the exercise in *Section Error! Reference source not found.* with the following exceptions:

- The dimensions of the lattice are 4x4x3 rather than 5x5x3. Because of this, the fill indices are now -1:2 rather than -2:2 in the x direction. The same is true in the y direction.

- The dimensions of the bounding box are changed from approximately 250x250x300 to approximately 200x200x300. This change was made so that a four element array would fill the box without adjusting the pitch.
- The spheres of beryllium and aluminum kept the same radius and center but are represented as an s surface with four parameters rather than a so surface. This was done to simplify moving the center point off the origin in the discussion to follow.

The input file for this example is as shown below:

```

c      Created on: Tuesday, October 03, 2006 at 09:31
1      0      -5 2 -1 6 -3 4 fill=9
2      0      5 :-2 :1 :-6 :3 :-4
3      0      -7 8 -9 10 -11 12 u=9 lat=1 $ROW 1
      fill=-1:2 -1:2 -1:1
      5 5 5 3 $ROW 1
      5 5 5 3 $ROW 2
      5 5 5 3 $ROW 3
      5 5 5 3 $ROW 4
      5 5 5 3 $ROW 1
      5 5 5 3 $ROW 2
      5 5 5 3 $ROW 3
      5 5 5 3 $ROW 4
      5 5 5 3 $ROW 1
      5 5 5 3 $ROW 2
      5 5 5 3 $ROW 3
      5 5 5 3 $ROW 4
4      212    -1.85 -13 u=3
5      0      13 u=3
6      208   -2.699 -14 u=5
7      0      14 u=5

1      px 99.9
2      px -99.9
3      py 99.9
4      py -99.9
5      pz 149.9
6      pz -149.9
7      px 25
8      px -25
9      py 25
10     py -25
11     pz 50
12     pz -50
13     s 0 0 0 10
14     s 0 0 0 20

mode N
m212 4009.60c      -1 $beryllium metal
m208 13027.60c     -1 $aluminum
imp:N 1 0 1 4r $ 1, 7
print
sdef x=15 y=0 z=0
nps 1000

```

For this lattice with an even number of elements, the center of the (0,0,0) element must be moved to the upper right corner (in x and y). To move the center of the (0,0,0) element after the lattice has already been created, the surfaces defining the lattice must be moved by half the width of the lattice element. In this case, because the pitch is 50, surfaces 7 through 10 must have 25 subtracted from them. Surfaces 11 and 12 do not need to be modified because the lattice is only being moved in x and y.

In the Input window, make the following changes.

Change surface 7 to: px 0

Change surface 8 to: px -50

Change surface 9 to: py 0

Change surface 10 to: py -50

On the Input Window, **Click Save...Update.**

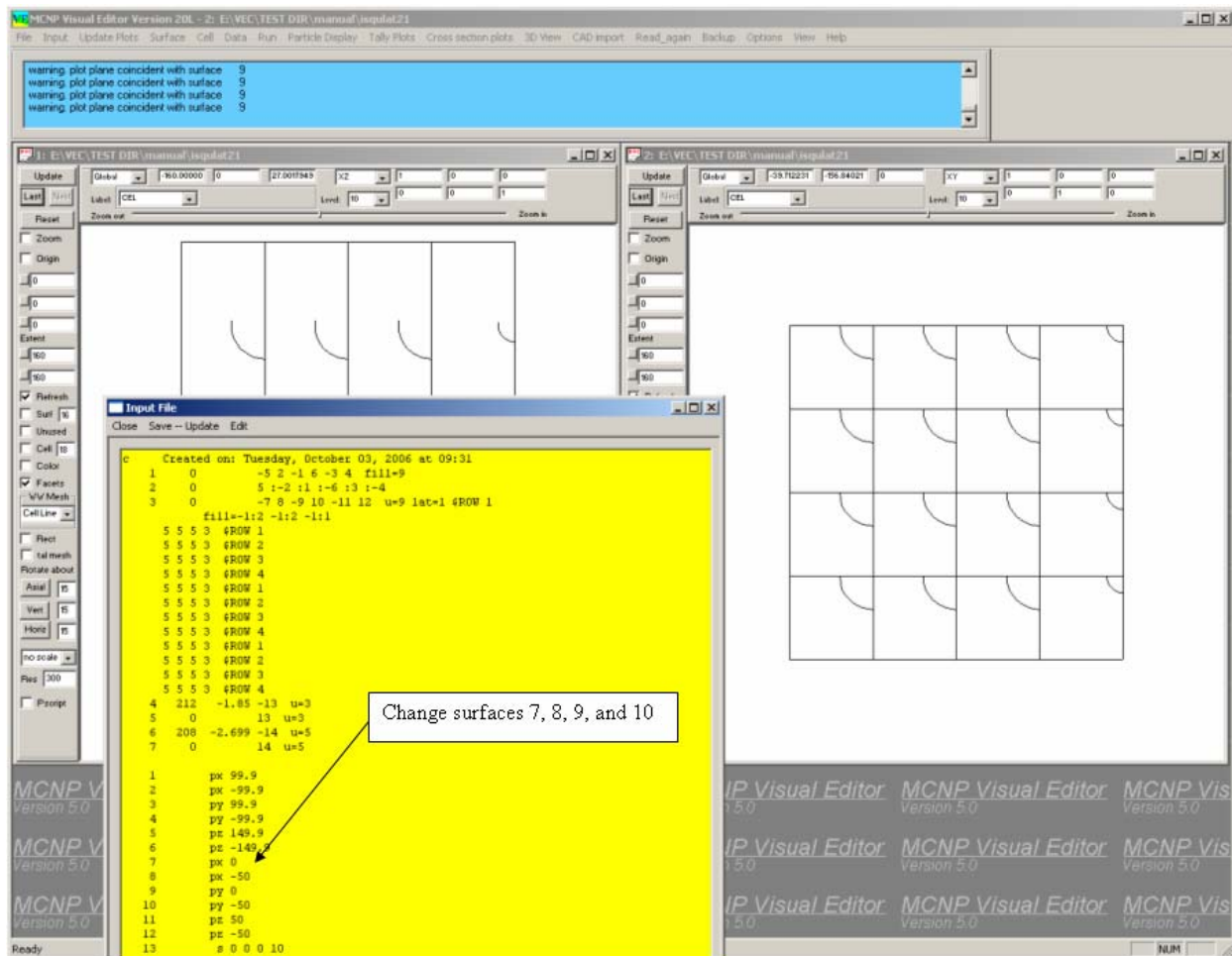


Figure Error! No text of specified style in document.-2 Display with Lattice Center Moved to Lower Left

The lattice has moved but the inner spheres have not. They also need to be translated. To move the inner spheres, make the following changes:

Change surface 13 to: s -25 -25 0 10

Change surface 14 to: s -25 -25 0 20

This changes the center point for the sphere to a point at (-25, -25, 0) which is the new center of lattice element (0,0,0).

On the Input Window, **Click Save...Update**

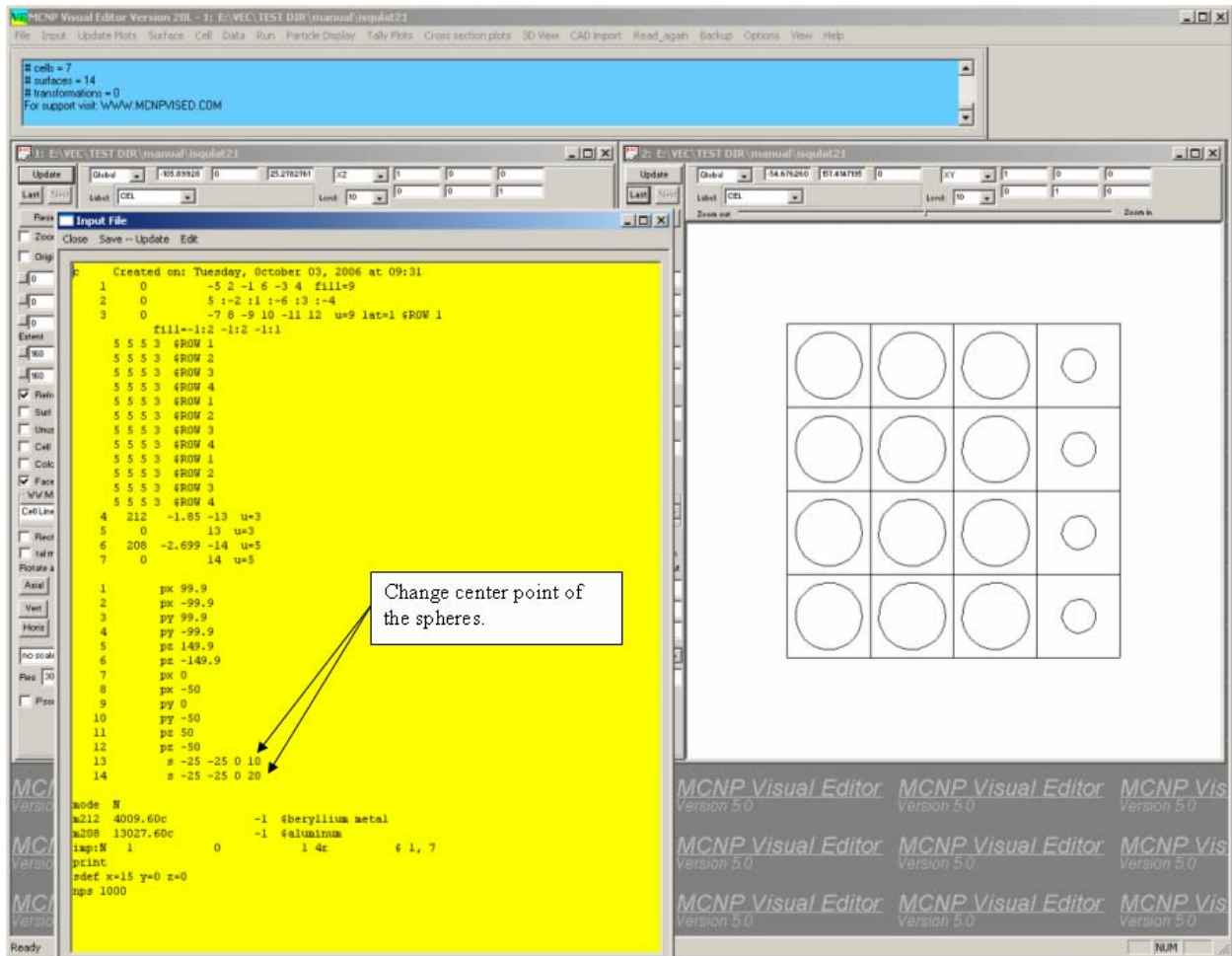


Figure Error! No text of specified style in document.-3 Lattice with Sphere Origins Modified.

Figure Error! No text of specified style in document.-3 shows the lattice with the spheres properly repositioned.