1.0 Example: Moving the Center of An Existing Hexagonal Lattice

The example creating a 3d hexagonal lattice assumed the (0,0,0) lattice element was at the origin so in the above listing surfaces 4 and 5, 6 and 7, 8 and 9, 10 and 11 were created by the Visual Editor symmetric about the origin. This is often desired when the center of the lattice is the origin of the local universe being filled with this lattice. The spheres of surfaces 11 and 12 were centered about the origin because of this choice.

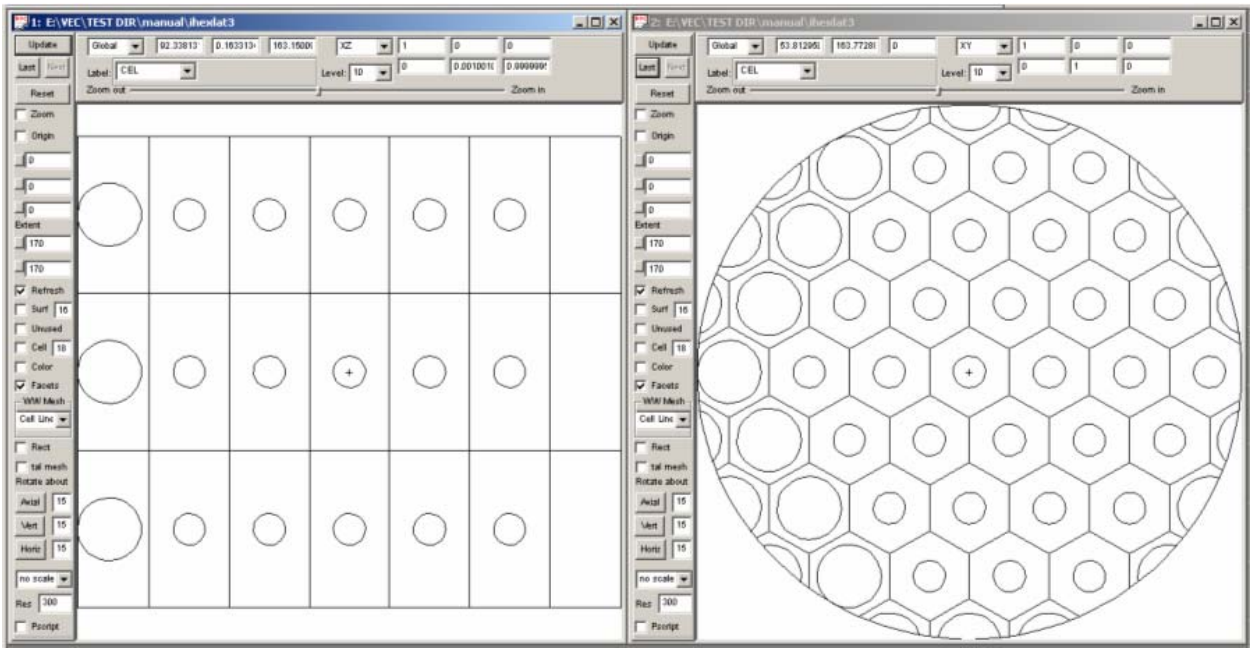

Figure 1-1 Off-Center Lattice

Figure 1-1 shows a hexagonal lattice with six elements across the x axis. Because there is an even number of elements, the lattice is not centered inside the bounding cylinder. To be centered, the center of the (0,0,0) element must be moved to the right side of the hexagon.

Start the **Visual Editor**.

Click on **File…Open…** and select the **ihexlat3** input file.

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

On both plot windows, **change both extents to 175**.

Figure 1-2 Changing the Basis Vector

On the Left plot window, change **the lower basis vector to be 0.01 in y and 0.999 in z.**

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:

- This lattice has 5 hexagonal rows rather than 4. Both have 3 axial rows. Because of this, the fill indices are now -4:4 rather than -3:3 in the x direction. The same is true in the y direction.
- The radius of the bounding cylinder was changed from 140 to 170. This was necessary to accommodate the larger lattice.

- The spheres of beryllium and aluminum kept the same radius and center but are represented as an sx surface with two 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: Thursday, October 05, 2006 at 12:13
    1     0         -2 -1 3  fill=9
    2     0         2 :1 :-3
    3     0         -4 5 -6 7 -8 9 -10 11  u=9 lat=2 $ROW 1
           fill=-4:4 -4:4 -1:1
      5 5 5 5 5 5 5 5 5  $ROW 1
       5 5 5 5 5 3 3 3 5  $ROW 2
        5 5 5 5 3 3 3 3 5  $ROW 3
         5 5 5 3 3 3 3 3 5  $ROW 4
          5 5 3 3 3 3 3 3 5  $ROW 5
           5 5 3 3 3 3 3 5 5  $ROW 6
            5 5 3 3 3 3 5 5 5  $ROW 7
             5 5 3 3 3 5 5 5 5  $ROW 8
              5 5 5 5 5 5 5 5 5  $ROW 9
      5 5 5 5 5 5 5 5 5  $ROW 1
       5 5 5 5 5 3 3 3 5  $ROW 2
        5 5 5 5 3 3 3 3 5  $ROW 3
         5 5 5 3 3 3 3 3 5  $ROW 4
          5 5 3 3 3 3 3 3 5  $ROW 5
           5 5 3 3 3 3 3 5 5  $ROW 6
            5 5 3 3 3 3 5 5 5  $ROW 7
             5 5 3 3 3 5 5 5 5  $ROW 8
              5 5 5 5 5 5 5 5 5  $ROW 9
      5 5 5 5 5 5 5 5 5  $ROW 1
       5 5 5 5 5 3 3 3 5  $ROW 2
        5 5 5 5 3 3 3 3 5  $ROW 3
         5 5 5 3 3 3 3 3 5  $ROW 4
          5 5 3 3 3 3 3 3 5  $ROW 5
           5 5 3 3 3 3 3 5 5  $ROW 6
            5 5 3 3 3 3 5 5 5  $ROW 7
             5 5 3 3 3 5 5 5 5  $ROW 8
              5 5 5 5 5 5 5 5 5  $ROW 9
    4   212   -1.85 -12  u=3
    5     0         12  u=3
    6   208  -2.699 -13  u=5
    7     0         13  u=5

    1        cz 170
    2        pz 149.99
    3        pz -149.99
    4        px 25
    5        px -25
    6         p 0.5 0.86602540378444 0 25
    7         p 0.5 0.86602540378444 0 -25
    8         p -0.5 0.86602540378444 0 25
    9         p -0.5 0.86602540378444 0 -25
   10        pz 50
   11        pz -50
   12        sx 0 10
   13        sx 0 20

mode  N
m208  13027.60c            -1  $aluminum
m212  4009.60c             -1  $beryllium metal
print
sdef x=50 y=0 z=0
nps  1000
```

To center the lattice, the center point of the (0,0,0) element must be moved so it is on the right edge of the current lattice. This involves translating the lattice center point by translating the six lattice surfaces and the center points of the spheres inside it by half the pitch of the lattice element. In this example, the pitch is 50 so the lattice must slide 25 centimeters to the left so that the lattice center is now on surface 4.

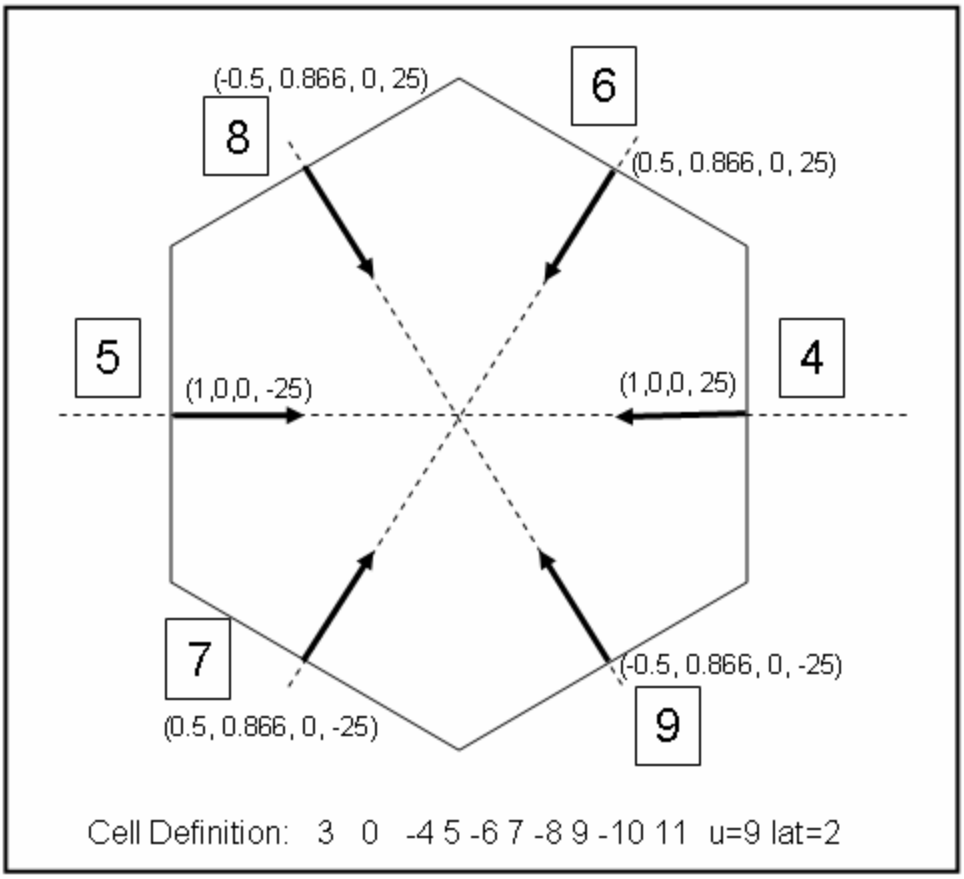

Figure 1-3 Translating the Center of the (0,0,0) Element

Slide surface 4 to the left by 25 centimeters so that it now goes through the center of the lattice. **Change surface 4** such that it is: **px 0**

Similarly, surface 5 must slide to the left by 25 centimeters. It is now 50 centimeters from the center of the lattice rather than 25.

Change surface 5 such that it is: **px-50**

Translating the general planes to the left is more complicated. The format of the general plane card is:

p A B C D

A, B, and C are the components of a (normalized) normal vector to the plane. These vectors are shown in *Figure 1-3* as dark arrows. The A, B, C, and D parameters for each surface are shown next to the surface in *Figure 1-3*. Because the plane is only sliding to the left and there is no change in rotation, A, B, and C stay the same.

D is the perpendicular distance from the plane to the origin (lattice center). Sliding the (0,0,0) element will change this parameter. Surfaces 4, 6, and 9 will be closer to the origin. Surfaces 5, 7, and 8 will be farther from the origin.

Currently, the card for surface 6 is: p 0.5 0.8660 0 25

In this card, D=25.

To translate this surface to the left by 25 centimeters, we take the dot product of the translation vector and the normal. This is added to the original value for D.

The translation vector is (-25, 0, 0) which is a vector pointing left with a magnitude of 25 centimeters.

The vector for the normal of surface 6 is given by the A, B, and C parameters or (0.5, 0.866, 0).

$$A \bullet B = (0.5,0.866,0) \bullet (-25,0,0) = -12.5$$

To calculate the new D value, add this to the current D value.

$$D_{new}=D_{old} + A \bullet B = 25 - 12.5 = 12.5$$

Change surface 6 such that it is: **p 0.5 0.86602540378444 0 12.5**

For surface 7,

$$A \bullet B = (0.5,0.866,0) \bullet (-25,0,0) = -12.5$$

To calculate the new D value, add this to the current D value.

$$D_{new}=D_{old} + A \bullet B = -25 - 12.5 = -37.5$$

Change surface 7 such that it is: **p 0.5 0.86602540378444 0 -37.5**

For surface 8,

$$A \bullet B = (-0.5,0.866,0) \bullet (-25,0,0) = 12.5$$

To calculate the new D value, add this to the current D value.

$$D_{new}=D_{old} + A \bullet B = 25 + 12.5 = 37.5$$

Change surface 8 such that it is: **p -0.5 0.86602540378444 0 37.5**

For surface 9,

$$A \bullet B = (-0.5,0.866,0) \bullet (-25,0,0) = 12.5$$

To calculate the new D value, add this to the current D value.

$$D_{new}=D_{old} + A \bullet B = -25 + 12.5 = -12.5$$

Change surface 9 such that it is: **p -0.5 0.86602540378444 0 -12.5**

Surfaces 10 and 11 do not change because the lattice is not being moved in the axial (z) direction.

Surface 12 defines one of the spheres in the lattice elements. It is shown as an sx surface. To shift it to the left by 25 cm change the x intercept (the first parameter) to -25.

Change surface 12 to be: **sx -25 10**

Similarly, **change surface 13** to be: **sx -25 20**

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

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