Positioning and Viewing Arrays in the Workbench

Introduction

This chapter covers how to position and view potential arrays in SIMION's **View** function's ion optics workbench. It is assumed that you have read the discussions of potential arrays in Chapter 2, 4, 5, and 6. If not, read the material before proceeding further.

Note: Chapter 8 covers how to fly ions within SIMION's ion optics workbench.

The first ten pages of this chapter present important conceptual information. Although the information density is quite high, you must eventually understand this material to use SIMION at its full power. ***Hang in there! You skip this information at your peril!***

The Ion Optics Workbench

SIMION 7.0 incorporates the concept of an ***ion optics workbench***. The workbench is an imaginary volume in space that you can size and project the ***images*** of potential arrays into. The workbench concept provides the framework to simulate a wide range of problems (*e.g. simple lens systems up to entire instruments*).

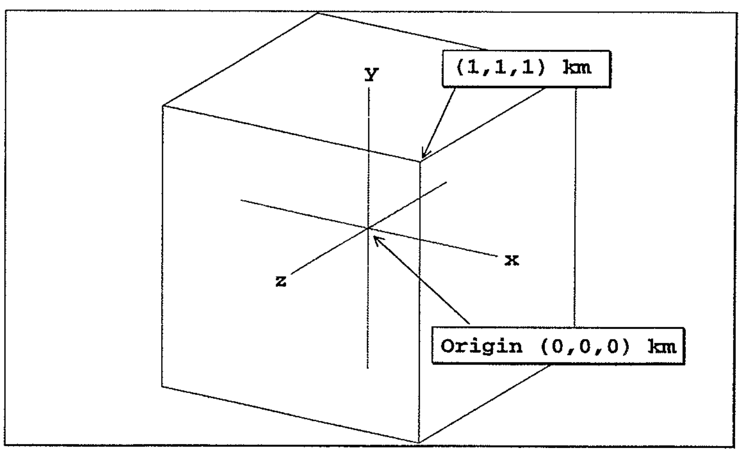


Figure 7-1 SIMION's 8 km^3 simulation universe

SIMION's Simulation Universe - a 8 km^3 Volume

SIMION's simulation universe is an imaginary 3D +/- 1 km cubic volume (*8 km^3 in volume*) with its origin (*x=0, y=0, z=0*) located in the center of the cube (*Figure 7-1 above*). The actual simulations are conducted within an ion optics workbench volume that ***must*** reside within the simulation universe.

Positioning and Viewing Arrays in the Workbench

SIMION's Ion Optics Workbench

SIMION's ion optics workbench *(or just workbench)* is an imaginary 3D rectangular volume of space ***within*** the simulation universe in which the actual simulations are conducted. All features (*e.g. array instances*) must be contained within the workbench. Moreover, ions must be created within the workbench to be flown, and any ion's trajectory that crosses a workbench boundary is terminated. ***Thus the workbench defines the limiting volume for a simulation***. You have the option of positioning and sizing the workbench volume anywhere within SIMION's simulation universe. ***This also implies that the maximum size allowed for the workbench volume is SIMION's simulation universe*** ($8\ km^3$). Workbench positions are ***always*** in mm relative to the origin of the simulation universe.

The Ion Optics Workbench .IOB Files

Workbench definitions are saved as **I**on **O**ptics work**B**ench - **.IOB** files (*e.g.* **EINZEL.IOB** *from the first demo flight - Appendix C*). An **.IOB** file contains definitions of the workbench volume, what arrays are required, their potentials, and where they are to be placed within the workbench volume. When you load an **.IOB** file *(from within* **View**) SIMION automatically loads any potential arrays that are required to support it. ***Saving the .IOB file is important because it conserves workbench definitions and/or changes between SIMION sessions***. Note: If you point the cursor to the View Status display panel object (*or Quit, IOB Load, and IOB Save buttons*) the name of the current **.IOB** file will appear in the display panel.

When an **.IOB** file is loaded by the **View** function, the workbench volume is recreated, all array instances are restored, all referenced potential arrays are loaded, and SIMION will ***optionally*** restore the potentials of all referenced **.PA** and **.PA0** files. SIMION can also automatically reload ion definition files (*.**FLY** or .**ION***), data recording files (*.**REC***), and kept ion trajectories (*.**KEPT_TRAJ***) that the user has elected to designate as auto-loading when the **.IOB** file was last saved.

Saving the .IOB file is important because it conserves workbench definitions and/or changes between SIMION sessions. It is recommended that you make extensive use of **.IOB** files. It is the most effective way to define, save, and restore a simulation project.

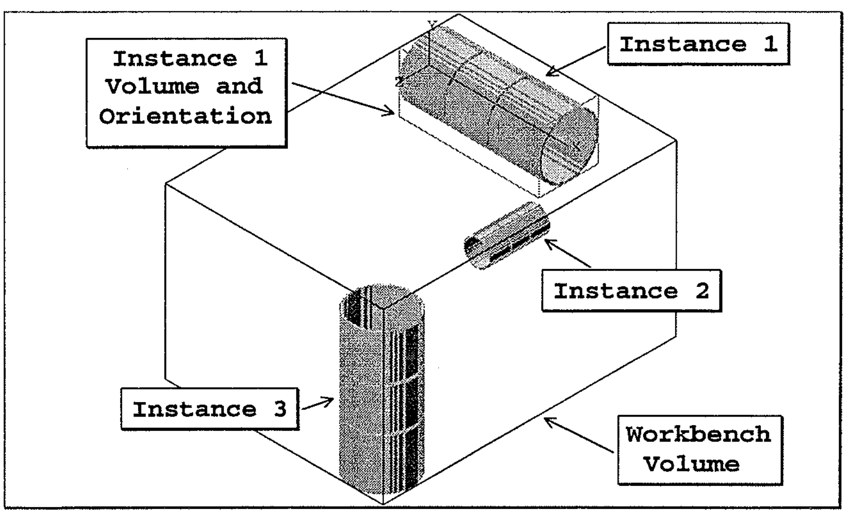


Figure 7-2 Projecting images of arrays into the workbench via array instances

The Projecting of Arrays into the Workbench via Instances

If we were asked to construct an image of an automobile in the workspace of our minds, we could describe one wheel of the automobile in great detail and then project images (*or instances*) of this wheel into the four wheel wells of the automobile. In the same manner, SIMION's array instance construct projects (*locates, scales, and orients*) the ***3D image*** of a ***single*** potential array into the workbench's volume taking into account the array's symmetry and mirroring attributes (*Figure 7-2*). The array ***instance*** construct provides the ***coupling*** between ***potential arrays*** in RAM ***and*** the virtual reality of the ***workbench volume*** where ions are actually flown. ***The array instance construct is very powerful and it is extremely important that you gain a solid understanding of it.***

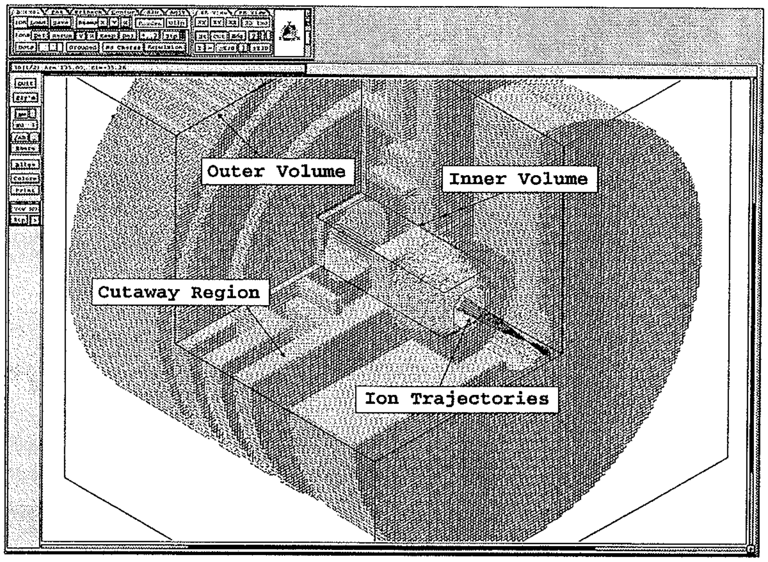


Figure 7-3 Cutaway view of a 2D cylindrical array projected as a 3D image by an array instance

Potential Arrays are Projected as 3D Objects

The projected potential array images in the workbench are always 3D. They represent the ***volume image*** of the potential array taking into account its ***symmetry*** (*planar or cylindrical*) and ***mirroring***.

SIMION visualizes an array by drawing x, y, and z lines (*in **array** coordinates*) that connect all electrode/pole points of the ***same*** potential. ***Projected array images appear to be constructed of small wire-frame cubes***. This particular rendering method makes arrays easy to visualize and allows SIMION to take advantage of powerful tricks to draw hidden line 3D images quickly (*Figure 7-3*).

How 2D Cylindrical Arrays Project

A 2D cylindrical array will appear as a ***cylindrical 3D volume*** when projected into the workbench via an array instance (*Figure 7-3*). If x mirroring is active, the 3D image will appear as two mirror-image cylinders joined at the x = 0 plane.

Note: While cylindrical arrays are surfaces of revolution, ***SIMION always visualizes them as if they were cylinders formed inside 3D planar arrays*** (*with wire-frame cubes*). This is ***only*** for display convenience. ***Although cylindrical apertures may not visualize as smooth circles, SIMION always treats them as smooth circles*** (*for fields and splats*) ***when flying ions through them***.

How 2D Planar Arrays Project

A 2D planar array will appear as a ***rectangular 3D solid***. Both x and/or y mirroring are allowed. Thus the 3D image may be mirrored across the x = 0 and/or y = 0 planes depending on the mirroring set for the potential array.

The 2D planar assumption implies an <u>infinite</u> extent in z. However, it is impractical as well as inappropriate to project images of 2D planar arrays in this manner. ***For visualization purposes, SIMION assumes <u>z mirroring is active</u> and that the array has a <u>minimum</u> z dimension of the y dimension of the array***. You have the option of ***increasing*** this z dimension (*by editing the instance definition*) to adjust the volume extent (*z depth*) of a 2D planar array (*e.g. for use in simulating the interior rod portions of a quadruple - see* **_QUAD** *demo*).

How 3D Planar Arrays Project

A 3D planar array will appear as a ***rectangular 3D solid***. Since x, y, and/or z mirroring are allowed, the 3D image may be mirrored across the x = 0, y = 0, and/or z = 0 planes depending on the mirroring set for the potential array. ***Thus an actual 3D planar potential array might define an eighth of a spherical shell** (centered at its origin)**; but if it were mirrored in x, y, and z; the visualized image would be a <u>complete</u> spherical shell.***

Details of the Array Instance Construct

An ***array instance***, in the SIMION context, acts to project a ***3D image*** of a potential array into a ***particular location, scale, and orientation*** within the workbench volume. Each instance projects ***one <u>and</u> only one*** potential array into ***one <u>and</u> only one*** location within the workbench.

The Workbench can have Multiple Instances

SIMION allows up to ***200*** instances to project images of potential arrays into a workbench volume. ***Thus up to 200 different potential arrays can be projected into a single workbench simulation.***

The ability to use multiple array instances is very powerful. It allows you to ***superimpose*** array instances of electrostatic and magnetic arrays to create volumes containing both electrostatic and magnetic fields. Moreover, array instances can be projected ***inside*** (*or more precisely* ***above*** *in priority*) other array instances to allow more detailed fields to be defined in specific regions. Each array instance has no knowledge of any other array instance (*all are blind to each other*). This means that the proximity of ***other*** array instances have ***absolutely no impact*** on the ***fields*** within an array instance. ***It is up to you to set the boundary conditions properly so that the fields make sense***. There is also a way to copy the 3D images of electrodes or poles from one array instance into the equivalent locations in another array instance (*via. The* ***Cpy*** *option*). This allows you to project the impact of one array instance into another, because you can **Refine** the resulting array.

It is important to remember that electrostatic and magnetic fields can only exist within the projected array instance images. Thus the workbench regions between array instances are ***<u>normally</u>*** assumed to be field free (*an exception for electrostatic field interpolations is discussed below*).

Two or More Instances can Reference the Same Potential Array

Two or more instances are allowed to project images of the <u>same</u> potential array. Figure 7-2 (*above*) shows ***three*** array instances of the ***<u>same</u>*** potential array (*an einzel lens*). Array instances can share the same potential array, because each array instance merely projects a 3D image of a potential array. As this example demonstrates, each array instance (*or image*) can be positioned, scaled and oriented independently. However, since all three array instances are projected images of the same potential array the electrode potentials of each array instance are identical, and the field gradients only differ by the relative scaling factors between the array instance definitions. Thus a single potential array can be used in several locations within the workbench (*e.g. one 90 degree spherical ESA instanced three times to simulate three identical spherical ESAs within the workbench volume*). ***This can save a lot of RAM because only one potential array in RAM is required to simulate several projected images.***

However, array instances projecting the same potential array are constrained as follows:

First, the ***potentials*** of ***all*** instances that project the ***same*** potential array will be ***identical***.

> **Note:** If you want to use a fast adjust potential array (**.PA0**) in two locations (*instances*), but want the adjustable electrodes/poles to have potentials that ***differ*** between the instances, you must make use of SIMION's multiple fast adjust base array capability (e.g. **.P?0** where **? = B-Z**).
>
> In this case you would return to the Main Menu Screen, save the current **.PA0** array as **.PB0**, reload the **.PA0**, return to **View**, Click the **PAs** Tab, select the instance for the **.PB0** array, click the **Rpl** button and select the **.PB0** file. Now the two instances are tied to ***different*** fast adjust arrays (*their potentials can now be different*). ***Be sure to save the workbench's .IOB file to remember the changes between sessions.***

Second, instance ***scale factors impact*** electrostatic and magnetic instances ***differently***.

- In the case of ***electrostatic arrays***, the electrostatic field gradients (*and thus ion accelerations*) are controlled by the instance scale factor. The ***smaller*** the projected image of the potential array, the ***stronger*** its field gradients (*assuming the same electrode potentials*). ***This is exactly what you would expect in the real world.***
- ***Instances of magnetic potential arrays are not impacted by scale factor.*** This is because the **Mag** (*the unit of magnetic potential used by SIMION*) is in units of **Gauss * Grid Units**. Thus its gradient (*Gauss*) is independent of instance scaling (*handy*). ***This was done because we normally think in terms of magnetic fields and not magnetic potentials.*** Thus SIMION's **Mag** conserves magnetic field strength (*makes magnetic fields independent of scaling factor*).

How an Instance Projects a Potential Array

Each active instance in the workbench is tied to a ***single*** potential array (*its RAM image*). The ***instance*** projects a 3D image of this potential array into the workbench volume by: ***Positioning, scaling, and orienting it.***

How Instance Images are Positioned

Instances are positioned based on ***three*** points of reference: The ***array's physical origin***, ***array's working origin***, and the ***currently aligned workbench origin***.

- The ***array's physical origin*** is the array's ***actual*** origin. For ***all*** arrays this is the array's 0,0,0 point in array grid units (*as you would see in the* **Modify** *function*).
- The ***array's working origin*** is the position within or near the 3D image of the potential array that you want to consider the origin for ***functional*** purposes (*e.g. for flying ions, array positioning/orientation, and etc.*). The ***array's working origin*** is ***always*** defined in terms of an ***offset*** in array grid units (*gu*) from the ***array's physical origin***.

  The default value for this offset is 0,0,0 (*or no offset*). ***This locates the working origin of the array at the physical origin of the array***. There are times when shifting the ***array's working origin*** away from its ***physical origin*** is helpful: To help position a 3D planar array that has a beam line that doesn't go through its physical origin (*common occurrence*), or to move the ***array's working origin*** to the ion emission point within the potential array (*facilitating the location of ion starting points*).
- The ***currently aligned workbench origin*** is the **0,0,0** point in workbench space (*mm*). ***Currently aligned*** means that the position of the ***workbench origin*** is either

unaligned (*normal – at the center of the simulation universe*) or ***aligned*** (*at the working origin of a selected instance*). The selective alignment of ***workbench coordinates*** is discussed later.

When an array is projected into the workbench, the instance combines the effects of ***two*** user defined ***offsets*** to position it:

1. The first, defines the ***offset*** of the ***array's working origin*** from ***currently aligned workbench origin*** in ***mm***. This offset is the principal way instances are positioned in the workbench volume.
2. The second, defines the ***offset*** of the ***array's working origin*** from its ***physical origin*** in ***grid units***. This offset is defaulted to **0,0,0**: Thus the ***array's working origin*** and the ***array's physical origin*** are defaulted to be the same.

How Instance Images are Scaled

Instance images of the potential array are scaled into workbench units (*mm*) via a user defined scale factor that has units of ***millimeters/grid unit*** (*mm/gu*). The ***default*** value for the scale factor is ***1.0 mm/gu*** (*one grid unit equals one mm of workbench distance*).

How Instance Images are Oriented

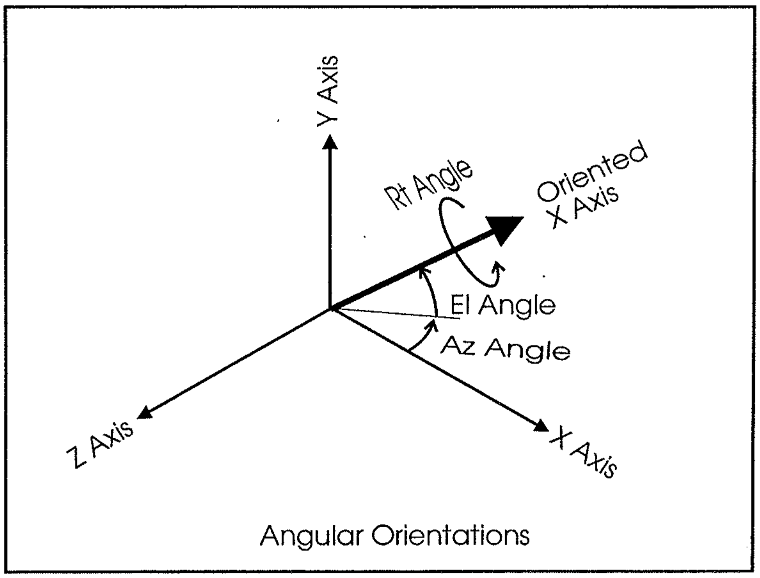


Figure 7-4 Angular orientation of instance relative to the currently aligned workbench coordinates.

Instances are oriented about their ***working origins*** by using three orientation angles (*Figure 7-4*): ***Az***, ***El***, and ***Rt*** (*in degrees*). These angles assume that the instance's x, y, and z axis are ***initially*** parallel to the ***currently aligned workbench coordinate x, y, and z axis*** respectively (*e.g.* **Az** = **El** = **Rt** = *0.0*). The angular orientations are performed in the following order:

1. The ***Rt*** angle defines the ***ccw*** rotation of the ***y-axis*** in the ***zy plane*** looking down the positive ***x-axis*** toward the array's ***working origin***.
2. The ***El*** angle defines the ***ccw*** rotation of the ***x-axis*** in the ***xy plane*** looking down the positive ***z-axis*** toward the array's ***working origin***.
3. The ***Az*** angle defines the ***ccw*** rotation of the ***x-axis*** in the ***xz plane*** looking down the positive ***y-axis*** toward the array's ***working origin***.

The Order of Instance Transforms

The above instance projection transformations are applied in the following order :

1. The ***array's working origin*** offset (**x,y,z** in **gu**) from its ***physical origin*** is applied first.
2. The rotation (**Rt**) transformation is applied second.
3. The elevation (**El**) transformation is applied third.
4. The azimuth (**Az**) transformation is applied fourth.
5. The scaling (**mm/gu**) transformation is applied fifth.
6. Finally, the ***array's working origin*** is offset (**x,y,z** in **mm**) from the ***currently aligned workbench coordinates*** to position the array instance within the workbench.

Integrally and Non-Integrally Aligned Instances

An instance can be either integrally or non-integrally aligned with the workbench. An integrally aligned instance has ***each*** projected array axis (*x, y, and z*) ***parallel*** to a workbench axis (*e.g. 0,0,0 or 90,0,-90 for* **Az**, **El**, *and* **Rt**).

Integrally aligned instances draw faster (*and better*), because SIMION's 3D rendering scheme is highly optimized for them. Features like potential energy surfaces require integral alignment. ***Thus you should strive to have as many of your instances integrally aligned as possible.***

SIMION provides an alternate method to define integrally aligned orientations based on which workbench axis the projected array's x and y axis are parallel to. If **Ax**, **El**, and **Rt** = **0,0,0** the orientations would be **x** = **+x** and **y** = **+y** (*the array's x axis points in workbench's +x axis direction and the array's y axis points in workbench's +y axis direction*). A second example, **90,0,-90** would give **x** = **-z** and **y** = **-x** (*the array's x axis points in the workbench's -z axis direction and the array's y axis points in the workbench's -x axis direction*). ***Selector objects are provided to allow you to select integral alignments in lieu of non-integral alignments.***

Note: ***Workbench coordinates*** can be ***temporarily*** aligned with any selected instance. This can be used to integrally align a non-integrally aligned instance for easier viewing or looking at its PE surface (*PE surfaces of instances require integral alignment*). Aligning ***workbench coordinates*** with any instance is discussed below.

Instances Can Overlap

Since we are dealing in virtual reality, PA instances can overlap (*share common volumes*). This enables both electrostatic and magnetic effects to be applied to the same volume. ***Please note: You must use common sense here. It is possible to carelessly model the physically impossible.*** If you have a combined electrostatic and magnetic problem, be sure to include the magnetic poles as electrostatic elements (*most likely at ground potential*) in your electrostatic array. ***Just because you overlap electrostatic and magnetic instances don't assume SIMION will automatically take into account the electrostatic effects implied by magnetic pole pieces*** (*it won't*).

Another use of overlapped instances is to position higher grid density (*more accurate*) instances within (*or more precisely **above** in priority*) lower grid density instances to improve accuracy in specific regions. This unfortunately introduces the problem of which instance to use in volumes where two or more of the same type (*e.g. electrostatic*) overlap (*in same volume*). ***The instance selection problem is solved by maintaining instances in an ordered numerical list*** (*below*).

Instances are Maintained in an Ordered List

SIMION maintains a numerically ordered list of all currently defined array instances. From the ordered list's prospective you can think of each instance as a ***layer***. ***The instance with the lowest number** (1) **is always on the bottom of the pile***. The instance with the higher numbers are stacked upon the pile in numerical order. ***The instance with the highest number is always on the top of the pile***.

The Significance of Instance List Order

Instance list order determines the electrostatic and magnetic fields that an ion sees and the electrodes it splats into when the ion is flying in a workbench region where instance volumes overlap. ***Instances with a higher instance number always have a higher use priority***.

Whenever SIMION is flying ions, it ***always*** starts at the ***top*** of the instance list (*highest instance number*) to search for instance(*s*) the ion is flying within. This search ***down*** the instance list (*top to bottom*) ***terminates*** after the ***first*** electrostatic ***and first*** magnetic instance containing the ion have been found (*first one of each type*). **Note:** To define a volume that has ***both*** electrostatic and magnetic fields, an electrostatic ***and*** a magnetic instance must both overlap in the volume's region.

When ions behave strangely and don't seem to be flying through the proper instance. ***Check the instance order***. There is a good chance that the ions ***may not*** be flying in the instance you think they are. ***Note: The Data Recording Option, discussed in Chapter 8, can be used to output the sequence of instance numbers an ion passes through.***

Changing Instance Order

The PAs Screen (*accessed via the* **PAs** *tab within* **View**) can be used to change an instance's location in the numerical instance list. Use the ***Instance Select*** panel to select the instance (*its image will be outlined in green*). Now click either the **Up 1** or the **Down 1** button to raise (**Up 1**) or lower (**Down 1**) the instance's priority in the number ordered list.

How Multiple Instances Interact

In two words - ***They Don't***. Each instance is an island. ***It has no knowledge of the existence of any other instance***. Thus an instance's fields are ***never changed*** by the proximity of another instance.

Transitions Between Instances

It is your responsibility to assure (*through appropriate boundary assumptions*) ***that there is appropriate field continuity in transitions between instances*** (*especially any that overlap*).

Interpolating Electrostatic Fields Between Instances

When an ion is flying between ***electrostatic*** instances (***outside of all electrostatic*** *instances*), SIMION checks forward and back along the ion's ***ballistic trajectory*** for intersections with an ***electrostatic*** source and destination instance. If intersections with ***electrostatic*** source ***and*** destination instances are found (*top to bottom instance list search*), the electrostatic potentials of the source and destination intersection points are determined and the potential gradient is calculated. ***Important: Any potential changes via User programs are ignored! This gradient can only accelerate*** (*or decelerate*) ***the ion along its ballistic trajectory*** (*no refraction - path bending*). ***Thus the ion will never see the effects of an electrostatic instance it is not on a collision path with***.

Copying Electrodes Into Base Array Instances

Even though array instances don't interact, you can copy electrode points between them so that the refining process estimates the fields more appropriately in 3D base array instances. The **Cpy** button on the PAs Control Screen can be used to accomplish this *(discussed later in this chapter).*

Aligning the Workbench Coordinates

SIMION treats the ***workbench coordinate*** system as the frame of reference in the workbench. However, there are times when it would be very convenient to be able to ***align*** the workbench coordinates, ***at least temporarily***, with the ***working origin*** (*and angular alignment*) of a particular instance. ***This can make viewing, measuring, instance adjustment/insertion much more direct.***

How to Align Workbench Coordinates with an Instance

This feature is supported via the **Align** button on the left edge of **View**. To temporarily ***align workbench coordinates*** with a particular instance, select the instance (*depress the* **PAs** *tab and use the* **Instance Number** *panel to select the instance number*), and ***then*** depress the **Align** Button.

When you ***align workbench coordinates*** with an instance, the ***workbench's origin*** will be positioned at the location of the instance's ***working origin*** and the ***workbench's x, y, and z axis*** will be ***aligned*** with the ***instance's x, y, and z axis*** (**Az** = **El** = **Rt** = *0.0*). ***All*** other active instances will have their positioning and orientation parameters automatically adjusted to reference the new ***aligned workbench coordinates***.

How to Restore Normal Workbench Alignment

To return to normal ***workbench coordinate*** alignment, click the **Align** button again (*to raise it*). ***All*** active instances will have their positioning and orientation parameters restored to reference the ***unaligned workbench coordinates***.

How to Retain a Workbench Coordinate Alignment Change

To make the current alignment of the ***workbench coordinates*** permanent, simply save its **.IOB** file (*using the* **Save** *button in the Normal Screen in* **View**). SIMION will ask if you want to make the current workbench alignment permanent.

Workbench Coordinate Alignment can be Changed at Anytime

You can change ***workbench coordinate*** alignment at any time (*even when ions are flying*). ***This allows you the maximum freedom to view, measure, and/or obfuscate whenever you please.***

Workbench Coordinate Alignment and SIMION Features

All features within SIMION ***automatically*** adjust for and use the ***currently aligned workbench coordinates*** as their frame of reference. These features are said to work with ***currently aligned workbench coordinates***.

The ***only*** feature that ***always*** uses ***unaligned workbench coordinates*** for its definition is the ***starting locations and directions of ions***. Whenever the ions' starting parameters are defined in ***workbench coordinates*** (*they are usually defined in a selected instance's coordinates*), these parameters are assumed to be in ***unaligned workbench coordinates***. This prevents you from having to change the starting locations and directions of your ions just because the **Align** button is depressed. SIMION will ***automatically*** translate the ions' starting locations and directions into the ***currently aligned workbench coordinates***.

The Default Workbench

If you enter **View** with a non-empty potential array selected, SIMION will first check to see if this array is referenced in its current workbench definition (**.IOB** *image*). ***If not, it will automatically create the following default workbench for the potential array:***

Positioning and Viewing Arrays in the Workbench

1. A ***3D image*** of the potential array will be projected into the workbench volume via a default array instance definition.
   - The array instance will position the ***array's physical origin*** at the workbench origin.
   - The array instance will project the array image with a scale factor of ***1.0 mm/gu*** (*1.0 workbench millimeter / array grid unit*).
   - The array instance will ***align*** each projected array image axis with its equivalent workbench axis (e.g. instance's x-axis aligned with workbench's x-axis: **Az** = **El** = **Rt** = *0.0*).
2. The workbench volume will then be minimized to just contain the array instance's projected array image (*by using workbench dimensions in **integral** mm*).

The default workbench simulates what users of pre 6.0 versions of SIMION have seen in the **View** function. However, it is important to realize that SIMION 7.0 ***never*** enters **View** without having an active workbench definition (*either pre-existing or by default assumption*). For example, in the Chapter 2 SIMION demonstration, an workbench definition was automatically created with a defaulted instance projecting **test.pa0** as described above when the **View** function was entered with the **test.pa0** potential array selected.

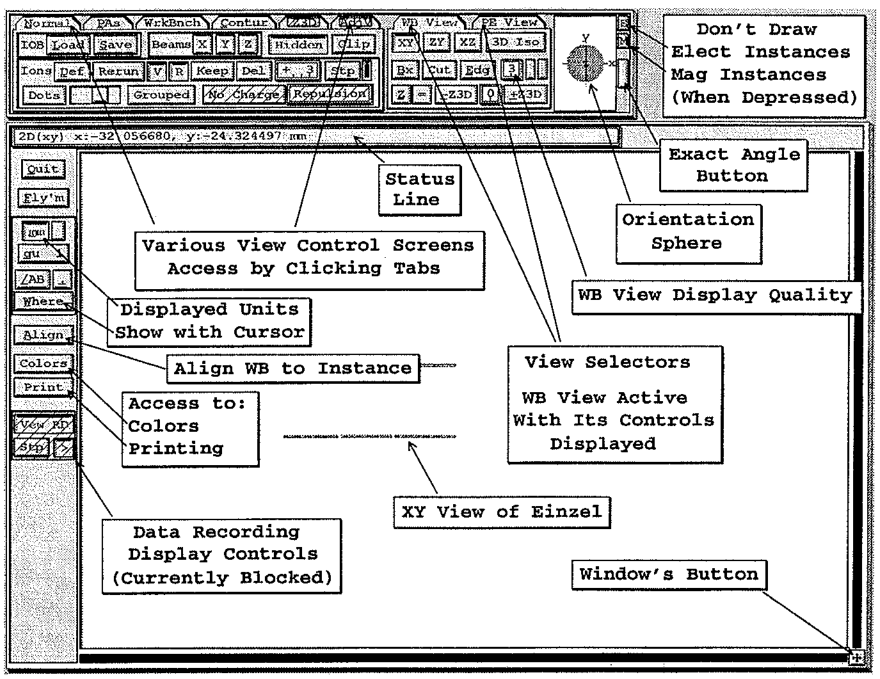


Figure 7-5 Image of View Screen with Einzel lens displayed and selected features annotated

Accessing SIMION's View Function

Now that you have waded through ***all*** this preliminary material, you are prepared to get into the ***View*** function and flail about (Figure 7-5). Use one of the following recommended approaches for entering ***View*** from the Main Menu Screen:

Entering View With a Potential Array

Select the desired potential array (*make sure its button in depressed*) and then click the **View** button or hit the **V** key. If the selected potential array is instanced in the current workbench, SIMION will re-enter that workbench. Otherwise, SIMION will create a default workbench definition for the file (*as discussed above*) and enter **View**.

Entering View With an .IOB File

It is suggested that you click the **Remove All PAs From RAM** button before loading a new **.IOB** file (*to remove RAM clutter*). Enter **View** without selecting a potential array (**Empty PA** *button is depressed*). SIMION's GUI File Manager will assist you in selecting an **.IOB** definition file (*e.g.* **EINZEL.IOB**). You should switch to the desired project directory (*click on it - if not currently selected*) and click ***both*** mouse buttons on the selected **.IOB** file name. SIMION will load the **.IOB** file and its referenced potential arrays. It will also ask you if you want ***all*** array potentials restored to what they were when the **.IOB** file was saved (*works for* **.PA** *and* **.PA0** *arrays*). Normally, you should click ***Yes*** (*the default*). SIMION will also ask if it should automatically reload ion definition files (*.**FLY** or .**ION***) and data recording files (*.**REC***) that the user has elected to designate as auto-loading when the **.IOB** file was last saved. Any kept ion trajectory files (*.**KEPT_TRAJ***) will be automatically loaded too.

A Tour Around View 's Screen

Figure 7-5 above shows a sample image of **View's** screen. Controls are located on the left edge and at the top. The currently selected view is displayed in the window. ***Note: SIMION <u>automatically</u> blocks access to screens as well as individual controls whenever their use would be inappropriate.*** In general, most features are accessible even when ions are flying. The objective is to make the **View** function as interactive as possible.

The Controls at the Top of the Screen

There are three groups of control screens at the top of the View Screen: A group of six control screens, a group of two view control screens, and finally an orientation sphere with three view control buttons.

The Six Control Screens Group

The group of six control screens are located in the upper left corner of the display. They are organized as six tabbed folders (*the Normal Screen is currently on top*). The six control screens are:

Normal	Controls for **.IOB** file saving and loading, instance axis beams, hidden line controls, and ion flying controls.
PAs	Controls to create, select, modify, and edit instances.
WrkBnch	Controls for displaying/changing the workbench size.
Contur	Controls for drawing potential and/or gradient contours.
Z3D	Controls for displaying/changing size of current 3D zoom volume. ***Access blocked if not currently 3D zoomed.***
AdjV	Controls for displaying/adjusting user adjustable variables. These are defined in user programs (*Appendix I*). ***Access blocked if not currently flying ions with user programs active that have adjustable variables defined.***

The Two View Control Screens Group

Two view control screens are provided as tabbed folders as above (*the WB View Screen is currently on top*). ***A view type is selected by clicking its tab.***

WB View Controls for displaying workbench views including: Standard view buttons, box outlining, cutaway clipping, edge only viewing, display quality options, unequal 2D display scaling, and 2D/3D zooming.

PE View Controls for displaying potential energy surface views including: Surface polarity, box outlining, grid spacing, display quality options, 2D zooming, and surface relief.

The Orientation Sphere Group

The top rightmost group is composed of an orientation sphere and three display control buttons.

Orientation The orientation sphere displays/controls the orientation of the displayed view. Normally the sphere automatically swings to the nearest standard view. However, if ***exact angles*** are selected the orientation sphere can adjust the view orientation to the nearest degree.

Exact Angles The long thin button to the right of the orientation sphere selects exact angles when it is depressed.

E Button The **E** button turns off the displaying of all electrostatic instances when depressed.

M Button The **M** button turns of the displaying of all magnetic instances when depressed.

Controls on the Left Screen Edge

A collection of buttons are provided on the left edge of the View screen for various functions. These include quitting the **View** function, setting the displayed units, aligning the workbench coordinates, changing colors, printing the current view, and displaying the Data Monitoring Screen (*if active*).

Controlling the View

The **View** function supports both ***workbench*** (**WB**) and ***potential energy*** (**PE**) views. These views are accessed by clicking on their tab (*e.g.* **WB View** *for workbench view*). You can switch back and forth between **WB** and **PE** views even while ions are flying. The following material describes how to control what is shown in each of the two types of view.

Requesting and Halting View Re-drawing

The current view can be redrawn or the current re-draw can be halted at any time. Normally SIMION automatically re-draws the view when appropriate. However, you have the option of forcing the issue.

Requesting a Re-draw of the Current View

To re-draw the current view, move the cursor into the view area or to the orientation sphere and hit the **Enter** key (*to redraw entire screen while in SIMION hold down the* ***ALT*** *key and hit V*).

To Halt a Re-draw of the Current View

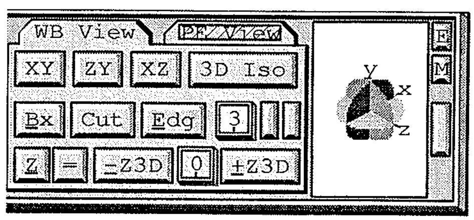
You can also abort a re-draw of the view at anytime by hitting the **Esc** key. Sometimes re-drawing a view can take quite a while (*e.g. display quality set to 9 in an exact angle WB view*). If the drawing is taking too long, hit the **Esc** key and then change the drawing parameters (*e.g. reduce the drawing quality or turn off exact angle drawing*).

Accessing and Controlling Workbench Views

Workbench (**WB**) views are accessed by clicking on the **WB View** Tab to access the WB View Control Screen (*displayed in Figure 7-5 above*).

What is Displayed in the WB View

In **WB View**, you are viewing a 3D volume within the workbench volume. Normally this is the ***entire*** workbench volume. ***However, you have the option of using a 10 level 3D zoom to limit your viewing to smaller volumes within the workbench volume.***



Controlling the Quality of the WB View

The WB View Control Screen has a panel object and two small buttons that can be used to control display quality.

The Display Quality Panel

The WB View Control Screen (*shown immediately above*) has a small panel object (*currently showing the number 3*). This **Display Quality** panel is used to control the quality of the displayed image (*and thus its drawing speed*). The number is adjustable from 0 (*lowest display quality*) to 9 (*highest display quality*). SIMION uses this ***number*** along with the ***projected size*** of each instance to determine how many vectors to draw to represent the instance. Thus when you zoom into an instance, SIMION will automatically draw it in greater detail.

The highest display quality setting (9) forces SIMION to draw ***all*** the instances' vectors no matter how big or small the instances' images appear on the screen. ***Warning: A display quality of 9 may result in very slow drawing in <u>exact angle</u> views*** (*discussed below*).

The Two Drawing Control Buttons

Just to the right of the **Display Quality** panel are two small buttons. SIMION visualizes instances via wire grid cubes. Sometimes a 3D isometric image can be made more definitive (*clearer*) when vectors in one direction are not drawn (*cubes require vectors drawn in three directions*). Each of these two buttons blocks drawing of vectors in a particular direction when depressed. ***You may find these buttons useful for seeing certain views more clearly.***

Controlling the Orientation of the WB View

SIMION provides three ways to control **WB View** orientation: Standard view buttons, an orientation sphere, and exact angle viewing. When the view orientation is changed any 2D zooming will be reset to full view. *Note: All orientations are relative to the currently aligned workbench coordinates.*

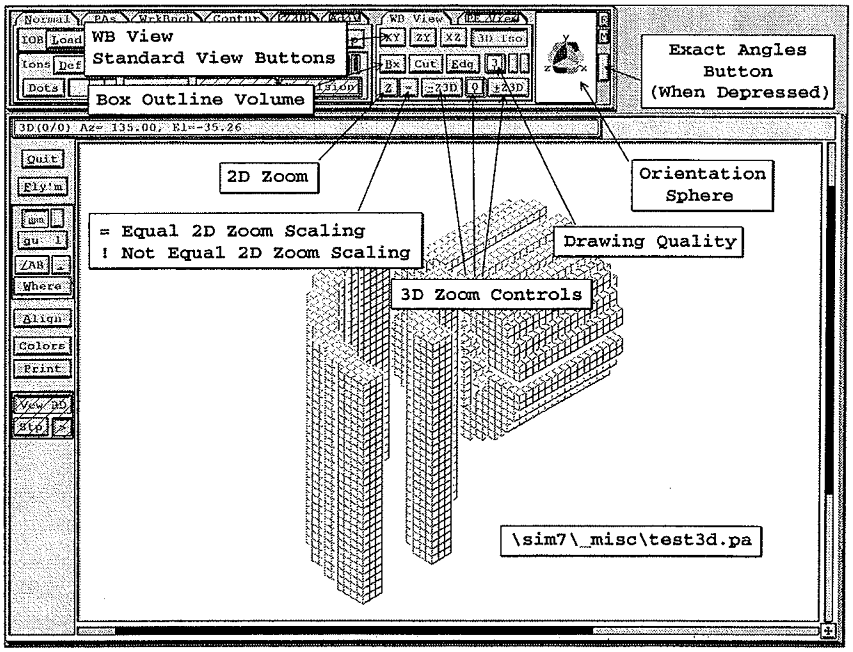


Figure 7-6 Workbench View Control Screen and its controls

Standard View Buttons

The WB View Control Screen has four standard view buttons (*Figure 7-6*): **XY**, **ZY**, **XZ**, and **3D Iso**. Clicking one of these buttons will access one of three standard 2D and one standard 3D isometric view. The orientation sphere will automatically track these orientations.

Using the Orientation Sphere - Standard Views

The orientation sphere (*to the right of the WB View Control Screen*) can also be used to set the orientation of the view. This is done by moving the cursor to the orientation sphere and ***dragging*** the sphere to the desired orientation with **either** mouse button depressed. The orientation sphere automatically swings to the ***nearest standard view*** when the mouse button is released.

The orientation sphere can access 12 standard 2D views and 8 standard 3D isometric views. ***It is recommended that you try to make used of standard views whenever possible because SIMION's instance rendering system is highly optimized for them.***

Note: Even though you are using a standard view, SIMION will ***only use fast rendering*** for those instances that are ***integrally aligned*** with the ***currently aligned workbench coordinates*** (*discussed above*). Any instance that is ***not integrally aligned*** will be rendered with the ***slower sampling based methods*** used with exact angle views. You can use the **Align** button to ***temporarily align*** the workbench coordinates with any selected non-integrally aligned instance (*speeding its display speed and improving its display quality*).

Exact Angle Views - Using the Orientation Sphere

If you depress the **long** button just to the right of the orientation sphere, SIMION will switch to exact angle views. The orientation object can then be rotated to the nearest one degree of azimuth and elevation angle (*Az and El angles will be displayed within the orientation sphere object*).

Note: The drawing speed and quality of the view will erode when exact angles are active (*in **WB Views** only - **not*** **PE Views**). This is because SIMION must use a ***slower sampling method*** for exact angle instance image rendering. To maintain speed, it automatically reduces the image quality. You can increase the value of the **Display Quality** number to restore quality. However, drawing can become quite slow for the higher numbers (*particularly at 9*). ***Remember, you can always hit the* Esc *key to halt drawing if things have become too slow.***

One trick is to use a display quality of 3 to quickly find the desired orientation, and then increase the drawing quality incrementally (*e.g. 5,6,7 and etc.*) until the rendering is the quality desired. This approach is generally the quickest way to find and display that special exact angle view.

Warning: Exact angle WB Views generate a lot of short vectors. Printing an exact angle **WB View** can swamp your printer's memory. Solution: Get more printer memory or don't print that exact angle **WB View**.

2D Zooming and Scrolling

SIMION provides several ways to 2D zoom and scroll the view. A 2D zoom merely magnifies the current view to help you see details. Scrolling moves the zoomed view about within the full view area.

2D Zooming Using Marked Areas

To 2D zoom (*magnify*), mark the area you want to zoom to (*drag a rectangle with the* **left** *mouse button depressed*) and then click the **right** mouse button (*or click* **Z2D** *button or hit the* **Z** *key*). To zoom back a level just click the **right** mouse button or **Z2D** button (*without marking*). To zoom back into a previous magnification hold down a **shift** key and click the **right** mouse button (*or click* **Z2D** *button*) ***Up to 10 levels of 2D zoom are remembered.***

To ***delete*** a 2D mark, move the cursor into the view area and hit the **Del** key.

Page View 2D Zooming and Scrolling

To page view 2D zoom, move the cursor to the window's button (*lower right corner of view*). Hold down the **right** mouse button. The screen will be redrawn full view with a cursor that surrounds the current zoomed area. Now hold down a **Ctrl** key and move the mouse (**right** *mouse button still depressed*). Notice that the size of the cursor marked zoom area changes.

To scroll, release the **Ctrl** key and move the mouse (**right** *mouse button still depressed*). Notice that the zoomed area now moves about within the view.

The **Ctrl** key can be depressed or released to instantly switch between zooming and scrolling as desired. Release the **right** mouse button when the desired area is marked and the view will zoom to it.

Current View 2D Zooming and Scrolling

To 2D zoom the current view, move the cursor to the window's button (*lower right corner of view*). Hold down the **left** mouse button. Now hold down a **Ctrl** key and move the mouse (**left** *mouse button still depressed*). Notice that the view can be zoomed in or out.

To scroll, release the **Ctrl** key and move the mouse (**left** *mouse button still depressed*). Notice that the view scrolls.

The **Ctrl** key can be depressed or released to instantly switch between zooming and scrolling as desired. Release the **left** mouse button when the desired area is displayed.

Note: You can speed up this process by ***also*** holding down the **right** mouse button. When the **right** mouse button is ***also*** depressed the view is quickly redrawn using box outlines for the instances. To glimpse the actual view, release the **right** mouse button ***momentarily*** and SIMION will re-draw the view.

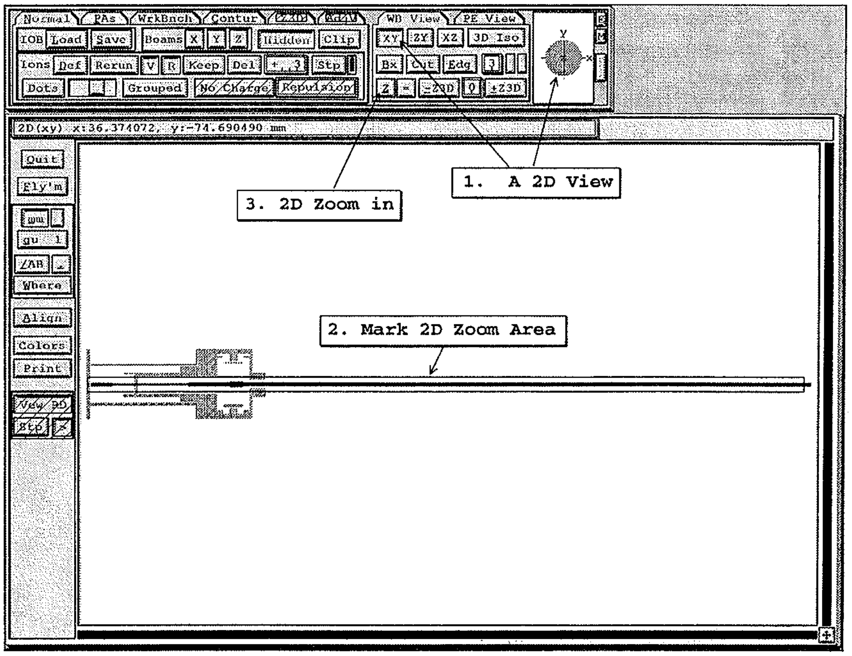


Figure 7-7 Steps in performing a 2D asymmetrical (*unequal xy scaling factor*) zoom

Unequal XY Scaling in 2D Zoomed Views *('=' Button)*

To the right of the **Z** button (*2D zoom*) is the '=' button that controls the symmetry of XY

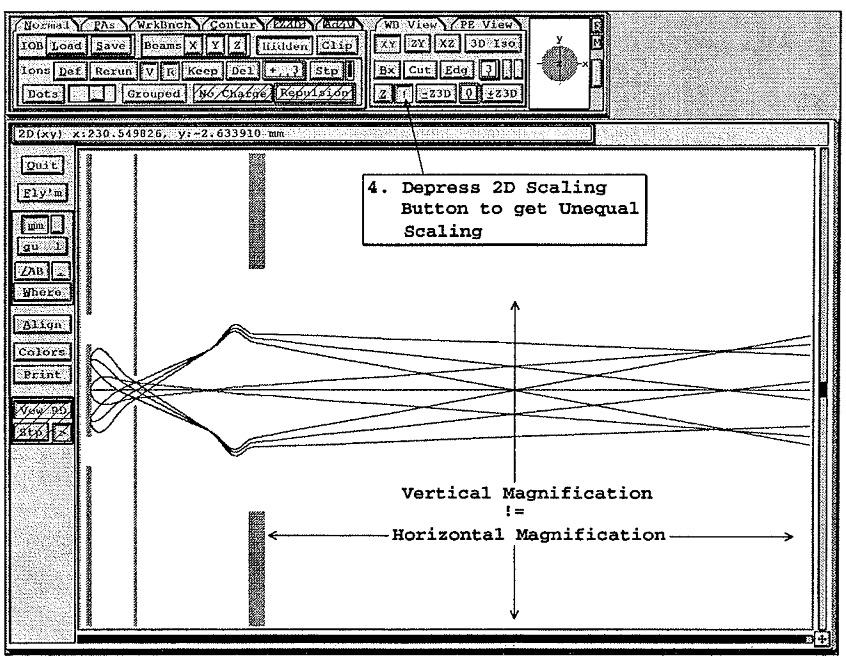


Figure 7-8 Example of using unequal xy scaling to better observe focusing in a narrow beam

scaling in 2D zoomed views (*Figure 7-7*). The default when entering View is equal XY scaling (*the button label displayed is an* '='). If the button is depressed it will change to a '!' label to indicate asymmetrical scaling is ***allowed*** in 2D Zoomed views (*Figure 7-8*). If you are looking at a 2D view (*not 3D or PE*) and have 2D zoomed in at ***least one level***, depressing this button (*changing it to* '!') will cause SIMION to asymmetrically scale X and Y so that the ***region marked when the zoom was made*** is ***stretched*** to the view boundaries. ***Each time you click this button the view will toggle between symmetrical and asymmetrical XY scaling.***

This feature is useful for viewing ion trajectories in long ion optics columns (*Figure 7-8*). You can use the zoom to expand the scale in y. ***Be careful, something may look quite wrong when it's highly distorted even though its really OK.***

Note: The Where function dimensions and Annotate dimensions remain correct with asymmetrical XY scaling active.

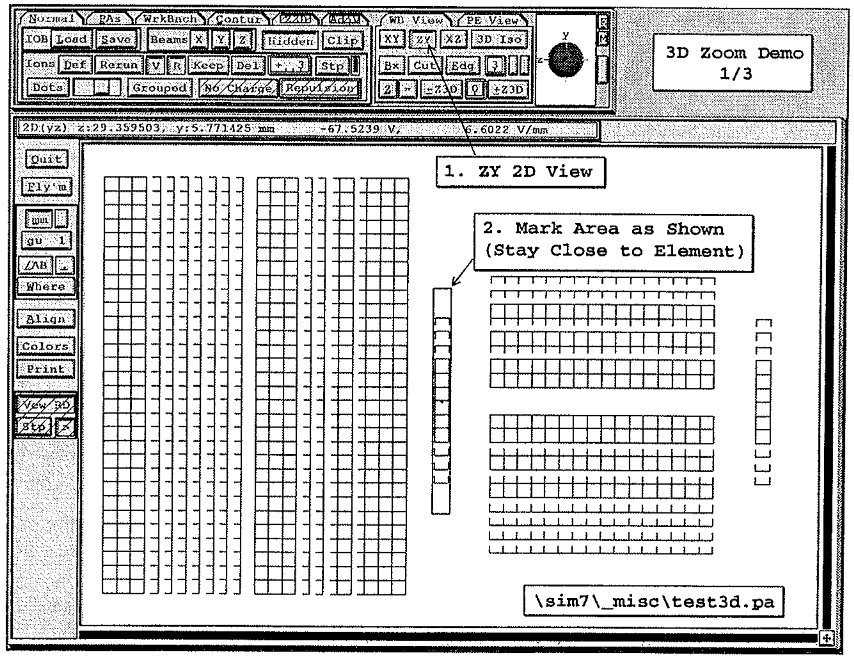


Figure 7-9 Demonstration of how to mark a volume and perform a 3D Zoom

Zooming the Volume - 3D Zooms

SIMION allows you to define volumes within volumes via a 3D zooming capability (*shown in Figures 7-9 to 7-11*). This feature is useful for limiting the size of the viewed volume. You can define a small volume (*e.g. exit aperture*), 3D zoom to it, and watch the ions fly through the volume.

Up to ten levels of ***bi-directional*** 3D zoom are supported. Each successive 3D zoom volume is contained ***within*** the preceding volume. The outermost level (*0*) is always the workbench volume itself. The term ***bi-directional*** means that the zoom volumes are remembered, and you can zoom in and out as appropriate.

The 3D Zoom Controls

The WB View Control Screen contains three objects that control 3D zooming: The **-Z3D** button, **Z3D Level** panel, and the **+Z3D** button.

Z3D Level This panel object displays/selects the current 3D zoom level (*currently displayed volume*). Level zero (*0*) displays the workbench volume. The panel can be used to change between 3D Zoom volumes (*if they are defined*).

-Z3D This button zooms back to the next outer zoom volume (*makes it the currently displayed volume*). Level zero (*0*) displays the outermost volume (*the workbench volume*).

+Z3D If a 3D volume is ***not*** currently marked, clicking this button zooms to the next inner 3D zoom volume (*if defined - else it beeps*).

If a 3D volume is currently marked (*see below*), clicking this button erases all 3D zoom volume definitions below the current level, and then uses the marked 3D volume to create a new 3D zoom volume, adds it to the zoom list, and makes it the current volume.

If the 3D zoom level is already at 9 (*maximum zoom*), the new 3D zoom volume replaces the one that was level 9.

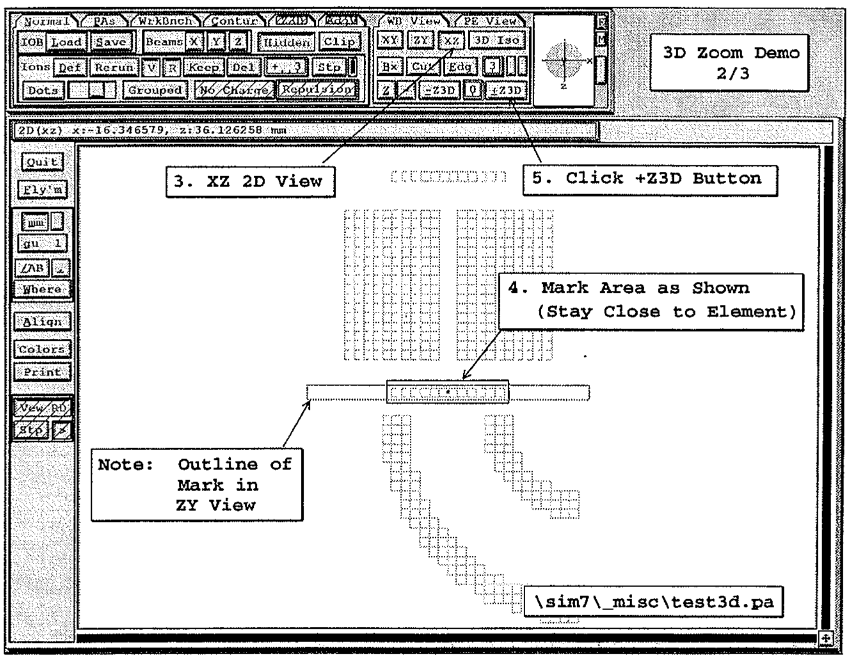


Figure 7-10 3D zoom demo showing how to further constrain a volume mark with additional 2D area marks

Marking a 3D Volume

View allows you to mark volumes in much the same manner as the **Modify** function (*Figures 7-9 to 7-11*). To mark a volume you must create your marks in ***standard angle*** (***not** exact angle*) ***2D views*** in the same manner you would mark for a 2D zoom. When you mark an area in a standard 2D view SIMION assumes the mark extends ***throughout the depth*** of the ***current volume*** (*it is a volume mark*).

Further, if you also mark in one or more of the ***two*** remaining 2D plane directions (*e.g. XY first, then ZY and/or XZ*), SIMION will assume each of these marks is a volume mark too. The actual resulting marked volume is the ***volume of intersection*** common to all of the volumes marked. ***If multiple 2D volume marks have no common intersection volume, SIMION will complain when you try to 3D Zoom.***

SIMION displays outlines of the volume represented by each mark. These marked volumes can be viewed using any standard 3D isometric view.

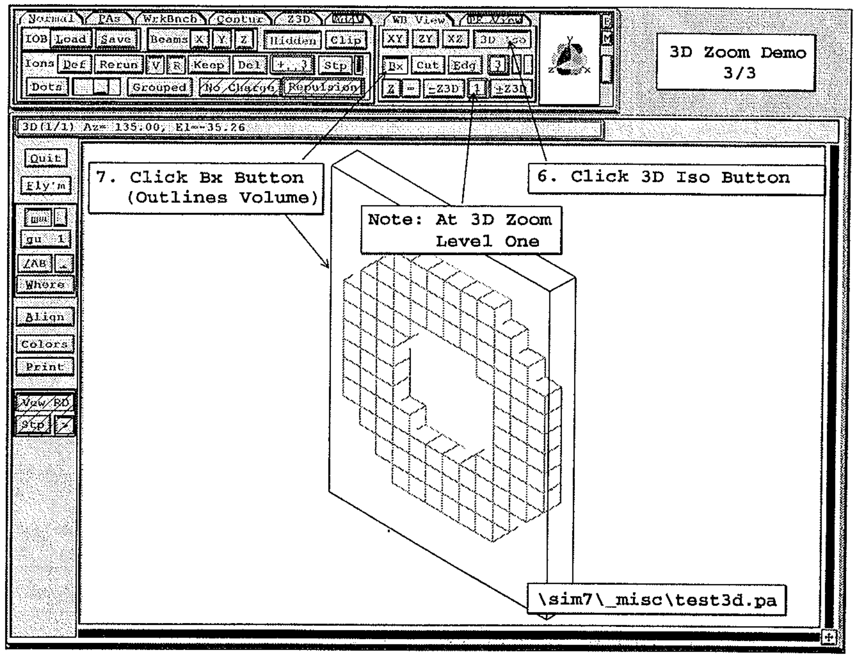


Figure 7-11 3D zoom demo showing the resulting volume zoom and how to outline its volume with a box

Deleting 3D Volume Mark(s)

Volume marks can be *deleted* by moving the cursor into the view area and hitting the **Del** key.

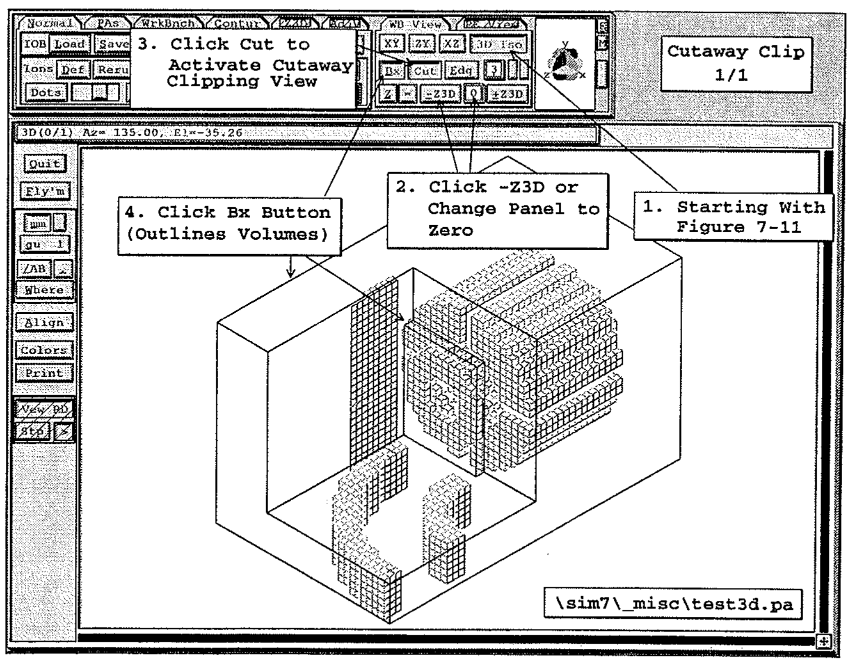


Figure 7-12 Example of using cutaway clipping to view a 3D zoom volume within its parent volume

Box Outlining

In figures 7-11 and 7-12 above, the **Bx** button was depressed to show the outline of the new 3D volume. Whenever the **Bx** button is depressed SIMION will automatically draw an outline of the current volume (*and the next inner volume if cutaway clipping is active - see below*).

Cutaway Clipping

It is sometimes very helpful to see an inner 3D volume displayed within its parent 3D volume in isometric 3D views (*e.g. see 3D zoom level 4 from within 3D zoom level 3*). The problem is that the parts of the outer volume can, and generally do, block the view of the inner volume. SIMION provides an option called cutaway clipping that cuts away part of the outer volume so that the inner volume is fully visible. SIMION changes what is cut away as you swing between isometric views.

To activate cutaway clipping click the **Cut** button (*so that it is depressed*). If an inner 3D

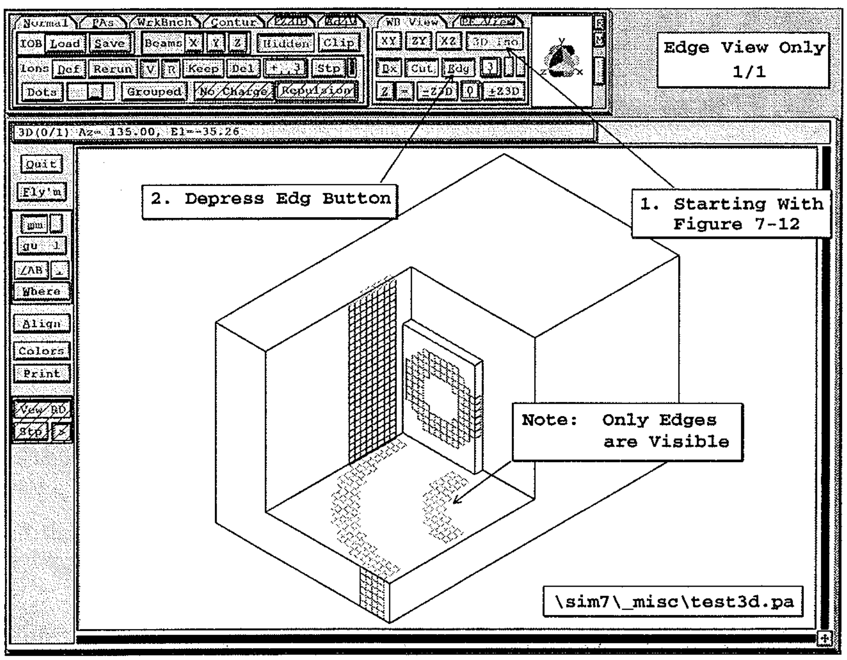


Figure 7-13 Example of the use of the edge only view option

volume is defined, SIMION will automatically cut away portions of it to make the inner volume visible (*Figure 7-12*). If the **Bx** button is depressed, the volumes and cuts will be outlined. ***If no inner volume is defined, the status of the Cut button will be ignored.***

Edge Only Views

Normally SIMION shows the interior of volumes (*normal and cutaway*). However, sometimes all you really want to see is the edge of the volume and what intersects it. When the **Edg** button is depressed SIMION only shows the edge vectors that intercept the edges (*Figure 7-13*).

The thickness of the edge boundary region can be adjusted by changing the **Drawing Quality** panel. The lower the quality (*e.g. 0*), the thicker the edge boundary region.

Note: Ion trajectories will appear as short line segments. If ion trajectories suddenly appear as dashed lines or are very short, you may have accidentally depressed the **Edg** button.

The **Edg** button is also used (*when depressed*) to signal to the PE View that PE surfaces of 2D cylindrical arrays should use the array's ***current*** 3D zoom volume boundary layer and not the array's center x-axis layer (*as is the default*).

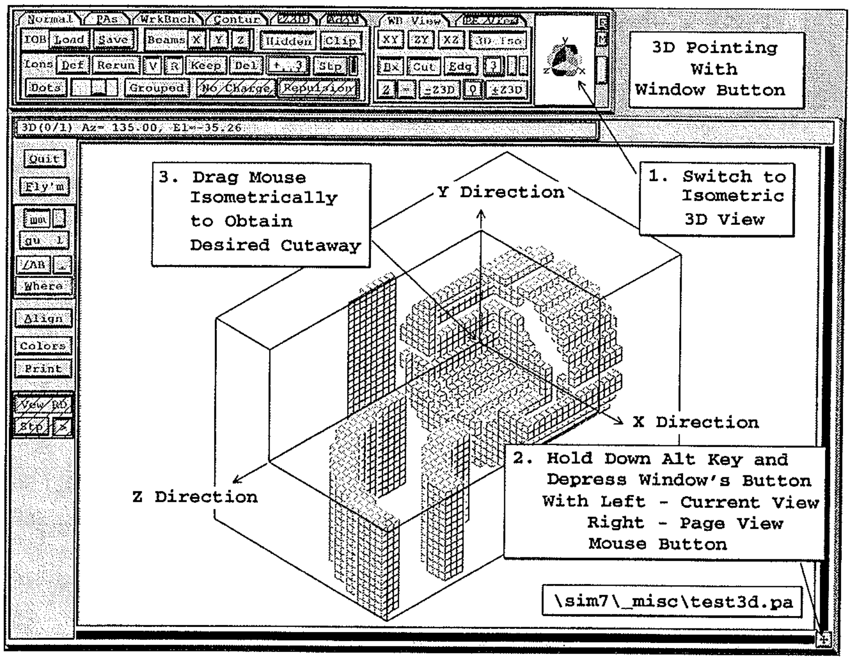


Figure 7-14 Example of creating a cutaway by 3D pointing

Using 3D Pointing to Create Inner Volumes

You have the option of using 3D pointing to create cutaways and inner volumes.

Creating a Cutaway by 3D Pointing

Figure 7-14 above, shows how to make use of 3D pointing to make a cutaway within the current volume (*current 3D zoom level*).

1. Swing to any ***standard angle*** isometric view.
2. Hold down the **Alt** key (*and keep it depressed*).
3. Move the cursor to the window's button (*lower right corner of view*) and depress the **right** mouse button for page view or the **left** mouse button for current view 3D pointing.
4. Drag the mouse in isometric directions (*e.g. vertical for y motions*) to move the cutaway point to the desired location.
5. You have the option of faster drawing if you depress the **other** mouse button too.
6. Release the mouse button(*s*) when you think you have cutaway what you want, and the view will be redrawn.
7. Repeat from step 2 until you cutaway what you want.

Creating an Inner Volume by 3D Pointing

Figure 7-15 below, shows how to create/size an inner volume via 3D pointing. You may start by either using 3D pointing to create a cutaway as in Figure 7-14 above, or with a existing inner volume displayed (*created by any means - e.g. marking and 3D zoom*) with the **Cut** button depressed.

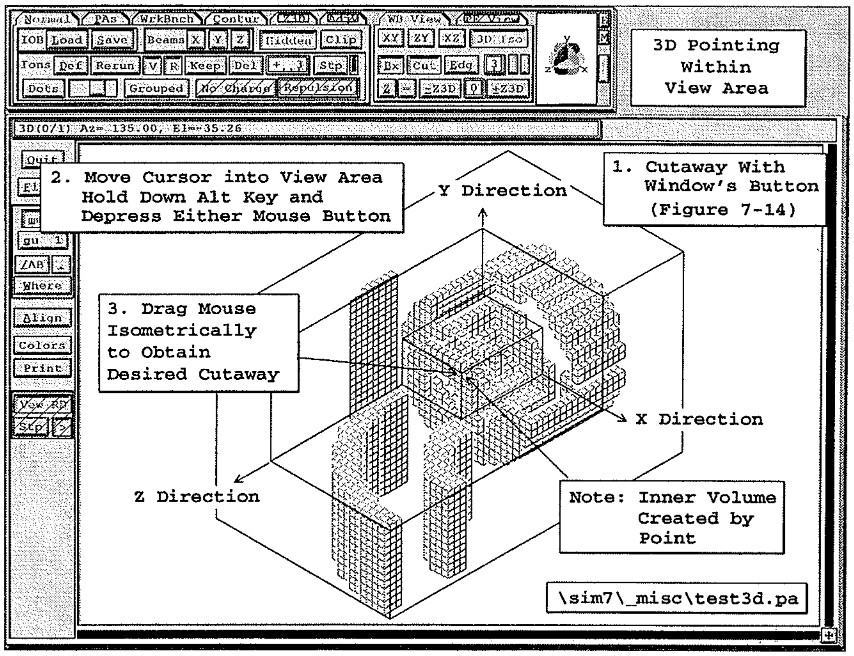


Figure 7-15 Example of creating/editing an inner volume definition by 3D pointing

1. Swing to any ***standard angle*** isometric view.
2. Hold down the **Alt** key (*and keep it depressed*).
3. Move the cursor into the view's area and depress **either** mouse button.
4. Drag the mouse in isometric directions (*e.g. vertical for y motions*) to move the inner volume corner point to the desired location.
5. You have the option of faster drawing if you depress the **other** mouse button too.
6. Release the mouse button(*s*) when you think you have the inner volume you want, and the view will be redrawn.
7. Repeat from step 2 until you have the desired inner volume. ***Note: You have the option of switching to any of the eight standard isometric views***. Thus you can move any of the inner volume's eight corner points (*just use the proper isometric view*).

Another Way to Adjust the Size of a 3D Zoom Volume

Once you have defined a 3D zoom volume you can adjust its size using the 3D pointing method discussed above or you can make use of the **Z3D** tab to access the 3D Volume Control Screen (*discussed later in this chapter*).

Using the E and M Drawing Control Buttons

Just to the right of the orientation sphere are two small buttons marked **E** and **M**. They can be used to suppress drawing of ***all*** electrostatic (**E**) and/or magnetic (**M**) instances when they are depressed. There are certain cases when this option is useful.

- You want to view electrostatic instance potential energy (*PE*) surfaces and not have magnetic instance PE surfaces confusing the issue (*depress the* **M** *button* ***before*** *entering PE View*).
- You want no instances drawn so you can see the ion trajectories more clearly (*depress both* **E** *and* **M**).

- You have a 3D surface contour and you want to see it without having the image of the instance blocking its view.

You also have the option of turning off the display of any instance individually via the PAs Control Screen (*discussed later in this chapter*).

Note: Although an instance may not be displayed, it doesn't mean that its effect is removed too! Ions fly through and splat into invisible (*not drawn*) instances just the same as when the instances are visible.

Accessing and Controlling Potential Energy Views

Potential Energy (**PE**) views are accessed by clicking on the **PE View** Tab to access the PE View Control Screen (*displayed in Figure 7-16 below*).

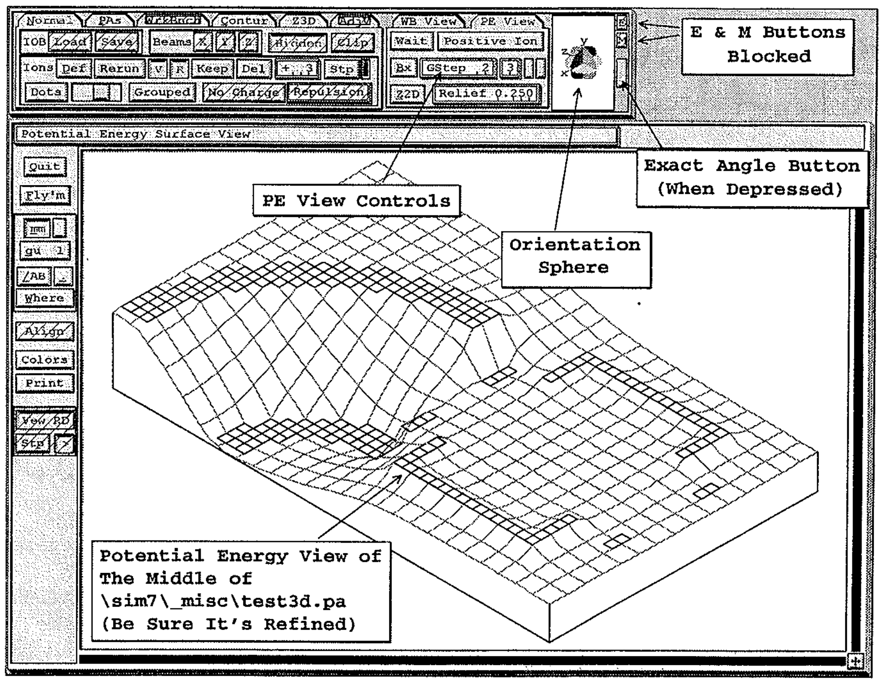


Figure 7-16 Potential energy view of an inside plane (*near the middle*) of \sim7_misc\test3d.pa

What is a PE View

In PE View, you are viewing a potential energy surface of ***one plane*** of the currently displayed 3D volume in the WB View. ***The potential energy surface has real physical significance for electrostatic instances***. A PE View of an electrostatic instance is to an ion what a miniature golf course is to a golf ball. Thus the PE View of an electrostatic instance is very useful for gaining insight concerning why the ions have the trajectories they do. Moreover, it provides an important level of understanding that can lead to design improvements.

Unfortunately potential energy views do not have much significance for magnetic instances. If your workbench contains both electrostatic and magnetic instances you may want to turn off the display of all magnetic instances (*by depressing the* **M** *button*) ***before*** clicking the **PE View** tab.

Special Requirements For Accessing PE Views

There are specific requirements that must be met before SIMION will allow access to PE Views and the display of specific instance PE surfaces.

Required WB Views for Accessing PE Views

SIMION will only allow access to potential energy views when the WB View is displaying a ***standard 2D view*** (*using either the three 2D view buttons or any 2D view of the orientation sphere*), and exact angle viewing is ***off*** (**Exact Angle** *button is not depressed*). SIMION will ***automatically*** block access to the **PE View** tab whenever, the current WB View is ***illegal*** for accessing a PE View.

Required Instance Alignment

To be displayed in a PE View, an instance must be ***integrally aligned*** with the ***currently aligned workbench coordinates***. An instance is integrally aligned if its x, y, and z axis are ***all parallel*** to ***any*** axis of the ***currently aligned workbench coordinates***. When an instance is integrally aligned a 2D view of the current workbench volume is a 2D view of the instance too. Thus SIMION can create a potential energy surface for it.

Note: the **Align** button can be used to ***integrally align*** the workbench coordinates with any instance (*thus allowing its PE surface to be displayed*). To temporarily align the workbench coordinates with a specific instance:

1. Click the **PAs** tab to access the PAs Control Screen.
2. Use the **Instance Selector** panel to select the desire instance. The currently selected instance's view image will be outlined in green.
3. ***Depress*** the **Align** button and the workbench coordinates will be ***temporarily*** integrally aligned with the selected instance's.
4. Now you can click the **PE View** tab and the instance's PE surface will be displayed.
5. Be sure to ***turn off*** this temporary alignment when no longer needed (*click the* **Align** *button to raise it*).

Instances Must be in the Current Volume to be Visible

To be visible in a PE View, an instance ***must be visible*** within the currently displayed WB View volume (*at the current 3D zoom level*). Instances that fall outside the current WB display volume ***will not be displayed*** in a PE View.

Only the portion of the instance that actually falls within the current WB display volume will appear in a PE View. ***This means that 3D volume zooms can be used to control the region of the instance that is displayed as a PE surface.***

What PE Surface Does SIMION Show?

When SIMION displays a PE surface, it is only displaying the PE surface of ***one layer*** of each integrally oriented instance that is visible within the current WB View volume. ***The question is: Which layer?*** The following explains the layer selections rules:

Rules for 2D and 3D Planar Instances

SIMION uses a simple layer selection rule for 2D and 3D Planar instances. Start inward from the front surface of the current WB View volume and display the first instance layer encountered. An instance layer is just like a layer in the **Modify** function (*a* ***plane*** *of array points*). ***SIMION always uses the plane array points nearest to the display screen for its selected PE surface layer.***

This means you can see the PE surfaces of layers inside an instance by cutting inside it with a 3D Zoom (*as in Figure 7-10 above*).

Rules for 2D Cylindrical Instances

2D cylindrical instances present a special problem for PE Views. What you normally want to see is the ***on x-axis layer*** (*central plane PE view*) assuming you're ***not*** looking at the instance from an end-on view. ***When the view of a 2D cylindrical instance is not an end-on view, SIMION shows the central plane (x-axis layer) PE view.***

If you want to view other layers of the volume in a ***side view*** of a 2D cylindrical array, click the **Edg** button before entering the PE View. ***SIMION now treats the 2D cylindrical array as if it were actually its pseudo equivalent 3D Planar dual for layer selection and PE surface generation.***

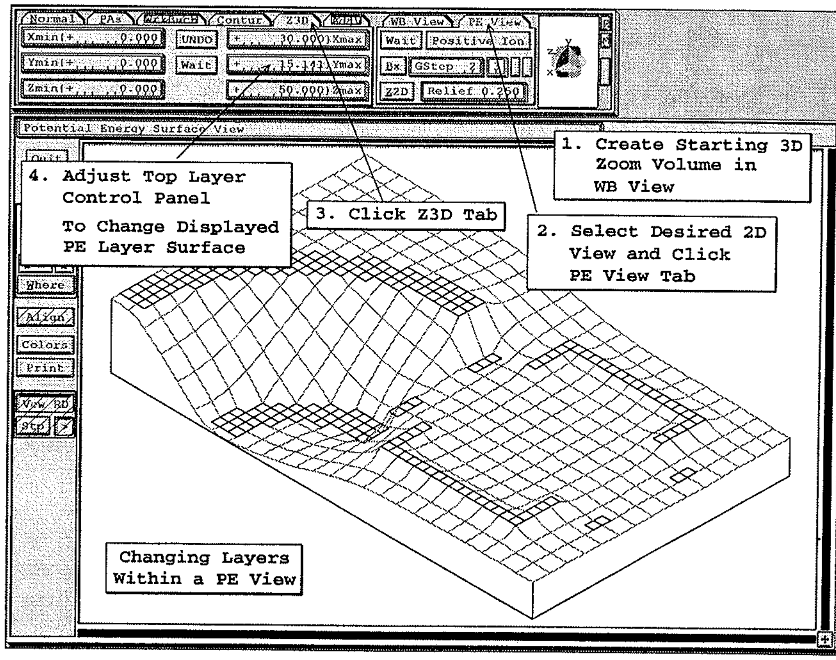


Figure 7-17 Example of using Z3D adjust screen to select PE display layers

Using 3D Zoom Tricks to Select PE Display Layers

As stated above, the 3D zoom feature of WB Views can be used to select which instance layer is viewed as a PE surface. However this approach is unsatisfactory if you want to change the displayed PE surface layer from within a PE View.

The trick is to 3D zoom into a starting volume and then enter the PE View. Now from within PE View click the **Z3D** tab to access the 3D Zoom Volume Control Screen. Change the position of the front of the 3D volume's surface (*using the **appropriate** panel control*) and SIMION will automatically re-draw new PE surface layers as required. Figure 7-17 shows an example of this.

The Various PE View Controls

The PE view controls consist of the orientation sphere, exact angle button, and other controls on the PE View Control Screen (*Figure 7-10 above*). When you switch between WB and PE views SIMION ***remembers the settings*** of these controls (*including orientation sphere and exact angles button*) and ***automatically restores them*** when you re-enter the view. The following material discusses the various PE View controls:

Orientation Sphere and Exact Angle Button

The orientation sphere works much the same way it did in WB Views. In the case of PE views there are only four standard views. These are the ***four isometric views*** with ***positive*** elevation angles.

If you want some other view, depress the exact angle button. You will then be allowed any view with a ***positive*** elevation angle. ***Note: The use of exact angles doesn't slow or complicate displays as it does in WB Views.***

Wait Button

The **Wait** button is provided to allow you to change several things without having SIMION automatically re-draw the PE view after each change. To stop auto-display updating ***depress*** the **Wait** button. ***Now make your changes***. Then click the **Wait** button ***again*** and the display will be updated.

Positive or Negative Ion Surfaces

SIMION provides a **Positive Ion/Negative Ion** button to display the potential energy surface that an ion of the selected charge polarity would see. ***This is very helpful to understand the differences in trajectories for ions of opposite polarities***. To select the desired surface polarity, click this button until it shows the desired ion polarity.

The Bx Button

The **Bx** button is used to display the outline of the current PE surface volume when depressed. This volume has the size of the 2D image of the current volume for its horizontal dimensions and the maximum potential for its vertical dimensions.

The GStep Panel

The **GStep** panel sets the grid spacing in terms of displayed electrode point spacing. The default value of 2, means draw one potential grid line (*green*) for every two drawn electrode lines (*black*). Higher values (*10 is the maximum*) result in a courser potential grid surface.

The Drawing Quality Panel

The next object to the right is the **Drawing Quality** panel. It has the same general function as the equivalent object in the WB View Control Screen. The default value is three. A display quality value of 9 forces all designated vectors to be drawn no matter how small the image of the instance on the screen. ***Note: Unlike the WB View the use of a drawing quality of 9 with exact angles will not adversely affect either drawing or printing speeds***.

The Two Small Buttons

Two small buttons are provided just to the right of the **Drawing Quality** panel. These buttons suppress the drawing of grid lines (*green*) in a particular direction (*when depressed*). SIMION will allow you to suppress drawing one, ***but not both***, directions of grid lines. ***Suppressing the drawing of grid lines in one direction sometimes improves the surface view***.

The Z2D Button

The **Z2D** button supports a ***10 level bi-directional 2D zoom*** in the same manner as in WB View. To zoom in, mark a 2D zoom area with the mouse (**left** *button depressed*); and zoom by clicking the **right** mouse button, clicking the **Z2D** button, or by hitting the **Z** key. Zoom outs are made by clicking the **right** mouse button (*or as above*) without marking an area first. To zoom back in, hold down the **shift** key and click the **right** mouse button (*or as above*) without marking an area first.

You also have the option to 2D zoom and scroll using the window's button in the same manner described for WB Views.

The Relief Panel

The **Relief** panel controls the vertical scaling factor or relief of the potential energy surface. Increasing the value for relief increases the y-height of the higher potential areas. The default value is 0.250. This is the control you make use of along with the orientation controls to obtain just the right vantage point.

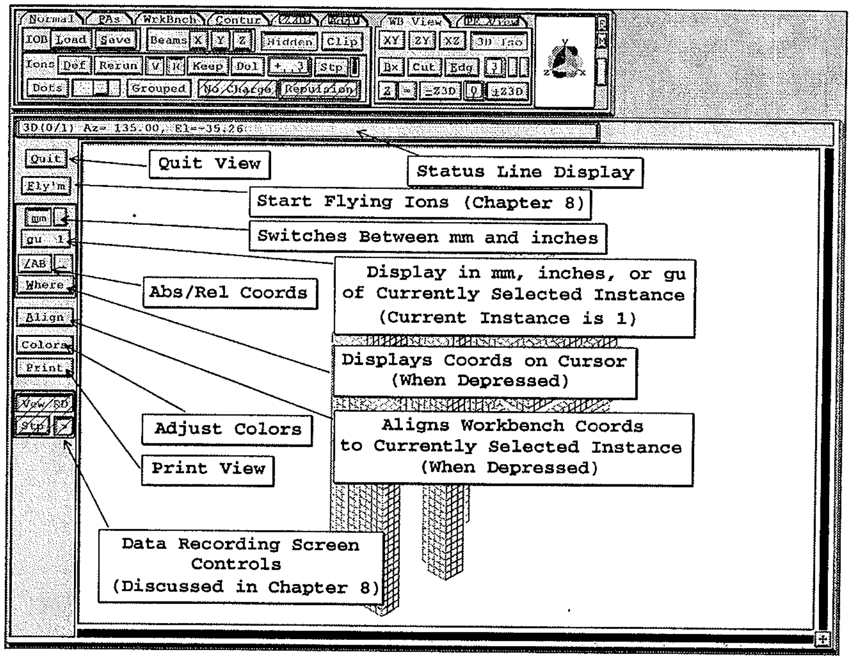


Figure 7-18 Annotated view of left edge controls

Controls on the Left Edge of the View Screen

The View Screen has a collection of controls on the left edge of the screen (*Figure 7-18 above*). Their functions will be described below:

The Quit Button

Clicking the **Quit** button or hitting the **Esc** key (*when ions are not currently flying and a screen re-draw is not currently in progress*) will signal to SIMION that you want to exit the **View** function. You will be asked if you're sure (*to prevent* **Esc** *happy exits*). Click **Yes** or hit the **Y** key and the current **View** session is history.

The Fly'm Button

Clicking the **Fly'm** button starts or terminates flying ions. See Chapter 8 for all the details.

The Status Line Display

The status line display shows various messages. If you place the cursor on it the IOB's name will be displayed. It is most frequently used for displaying cursor information within WB views (*doesn't display cursor information in PE Views*). What is displayed depends on the view:

Any 3D Isometric and All Exact Angle WB Views

The status line displays the azimuth and elevation orientation angles of the current view. ***If the cursor is over an electrode/pole, the potential of the electrode/pole will be displayed.***

Any Standard 2D WB View

The status line displays the absolute or relative 2D coordinates of the cursor in the current display units (*discussed below*). Moreover, if the cursor is over an instance the potential and gradient of the point under the cursor will be displayed. The feature displays the potential and gradient of the point on the first layer of the instance it encounters while looking inward from the screen. ***This works just like PE View layer selection*** (*discussed above*).

The Display Units Controls

Just below the **Fly'm** button is a group of buttons that control the units displayed on the status line and on the cursor (*when activated by the* **Where** *button*). Their functions will be discussed button by button:

The mm/in Button

The ***mm/in*** button when depressed forces the displayed units to be in **mm** or **inches** from the ***currently aligned*** ***workbench origin***.

The Blank Button

Just to the right of the **mm/in** button is a blank button. When this button is depressed, it switches the **mm/in** button (*if depressed*) from **mm** to **inches**.

Trick! When the **Where** button is depressed (*coordinates shown on cursor*), depress the **mm/in** button and point the cursor to a point on a 2D standard WB View. Let's say that the current display is in mm. Now hit the **Spacebar** without moving the mouse. The display is now in inches. ***Hitting the* Spacebar *toggles between inches and mm.***

The gu ? Button

The ***gu ?*** Button (**?** *is* **1** *in Figure 7-18*) designates that the displayed units be in grid units from the working origin of the currently selected instance. In Figure 7-18 the currently selected instance is 1.

To change the currently selected instance, click the **PAs** tab to access the PAs Control Screen. Now use the **Instance Selector** panel to designate the current instance number (*instance image in view will be outlined in green*). Finally, click the **Normal** tab to exit PAs Control Screen.

The /AB /RL Button

The **/AB /RL** button is used to toggle the coordinates displayed between absolute (*/AB*) and relative (*/RL*). The '/' key can be used to toggle this button from the keyboard. ***A construction line connects the cursor to the reference point when relative positions are active*** (*Whenever the button is depressed - /RL is displayed*). By default the relative reference point is the workbench origin. The '.' button (*discussed next*) is used to mark/edit relative reference points.

The . Button

The '.' button is used to record/change the reference point for relative positions. Use the mouse to mark the location of a reference point (*point to the desired location and click the left mouse button*). ***Note: Multi-2D view marking can be used to locate a 3D reference point.*** Now click the '.' button or hit the '.' key. A screen will appear with the coordinates of the marked reference point. You can edit these coordinates as desired and then accept them. If no point is marked when the '.' button is clicked or '.' key is pressed, the current reference point's screen will be displayed for you to view and/or edit.

The Where Button

When the **Where** button is depressed the absolute or relative coordinates of the cursor will be displayed on the cursor whenever the cursor is within a 2D standard angle WB View. The units displayed are selected via the unit controls described above.

The Align Button

The **Align** button is used to ***temporarily*** align the workbench coordinates with the working origin of the currently selected instance when depressed. ***This can be done at any time - even when ions are flying***.

How to Align the Workbench With an Instance

To align the workbench with an instance you must first select the desired instance (*the currently selected instance*) and ***then*** depress the **Align** button.

To select an instance, click the **PAs** tab to access the PAs Control Screen. Now use the **Instance Selector** panel to designate the current instance number (*instance image in view will be outlined in green*).

What is Changed?

When the workbench coordinates are aligned with an instance, the following changes are made:

- The workbench origin is located at the instance's working origin.
- The workbench x, y, and z axis are aligned with the instances x, y, and z axis respectively.
- The positions, scaling, and orientations of ***all*** other instances are changed to reflect the new workbench orientation.
- The coordinates of the current relative reference point are changed to reflect the new workbench orientation.
- The workbench dimensions are expanded, ***if needed,*** to contain the non-aligned workbench volume within the aligned workbench.

How to Return Back to Normal Alignment

The transformation can be reversed at any time by clicking the **Align** button (*raising it*). ***Note: All editing of instances done while the workbench is aligned with an instance: Adding, deleting, moving, sizing, and/or orienting will be conserved in the reverse transformation*** (*when the* **Align** *button is clicked again - to raise it*).

How to Make the Alignment Permanent

You also can keep the current alignment permanent by saving the current workbench definition to its current (*or create a new*) **.IOB** file. Click the **Normal** tab to access the Normal Controls Screen and click the **Save** Button. SIMION will ask if you want the **.IOB** saved with the current alignment. Click the **Yes** button and save the **.IOB** file. ***Both the saved*** **.IOB** ***file and current workbench image retain the alignment as the normal unaligned orientation.***

Uses for the Align Button

The following examples should serve to get you thinking of the many important uses of the **Align** button:

- To force an instance into integral alignment so that it can be viewed by WB View's fast rendering.
- To force an instance into integral alignment so that its PE surface can be seen in a PE View.
- To temporarily align on one instance so that positioning or orientation of another instance (*along perhaps an off-axis beam line*) can be more easily accomplished.

The Colors Button

The **Colors** button is provided to allow you quick access to SIMION's color palette controls. Changing colors can sometimes help improve visualization.

Note: There is also a **Colors** button on the Print Options Screen. It is provided to facilitate changing colors while printing.

The Print Button

The **Print** button accesses the print and annotate function to vector print the current view. ***See Appendix G for information on your printing options.***

Be sure to click the **Options** button to verify that the selected Windows printer and output orientation is appropriate. Remember! If you want color output, depress the ***B/W*** button so it will switch to the word **Color**.

Trick! If you want to pixel print the entire screen (*view and all*), hit the **<Ctrl F1>** key to access the GUI sketch/print utility, hit the **P** key for print, click the **NO** button and select full screen printing. Have Fun!

> Trick! If you want to pixel print the entire screen (*view and all*), hit the **<Ctrl F1>** key to access the GUI sketch/print utility, hit the **P** key for print, click the **NO** button to select full screen printing. Have Fun!

The Data Recording Display Screen Controls

The lowest area on the left of the view screen contains a collection of buttons used to control the Data Monitoring Screen (*when active*). Figure 7-19 below shows access to these controls as blocked. ***This* View *feature will be discussed in Chapter 8.***

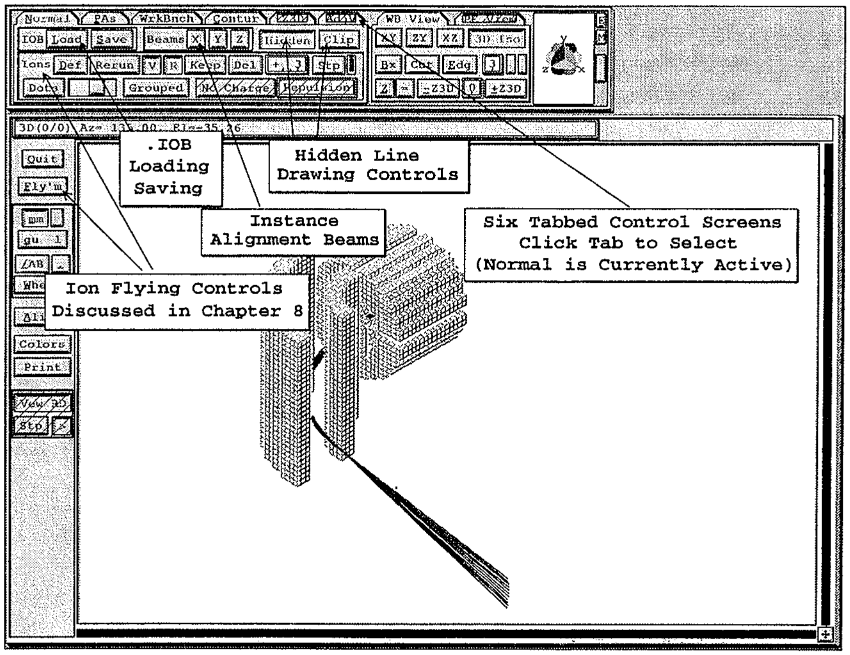


Figure 7-19 The six View control screens with the areas of the Normal control screen annotated

The Six View Control Screens

The final topics for discussion with the **View** function involve the six tabbed control screens: **Normal, PAs, Wrkbnch, Contur, Z3D**, and **AdjV** (*Figure 7-19 above*). Each of these control screens are accessed by clicking on their tab or hitting an access key (*e.g.* **N** *for* **Normal**) if allowed. Access to these control screens is normally allowed at any time, even when ions are flying. ***However, whenever access would be inappropriate, the access tab will automatically be blocked*** (*e.g.* **Z3D** *and* **AdjV** *tabs in Figure 7-19 above*).

The Normal Control Screen

The Normal Control Screen is accessed by either clicking the **Normal** tab or hitting the **N** key. Access to this control screen is allowed at any time. The Normal Control Screen provides access to **.IOB** file saving and loading, alignment beams, hidden line drawing controls, and the various ion flying controls (*discussed in Chapter 8*).

.IOB File Saving and Loading

The Normal Control Screen has **Save** and **Load** buttons for saving and loading **.IOB** files. An **.IOB** file contains a complete workbench definition: Workbench size, definition of active instances, the names of the potential arrays each instance references, and their potentials (**.PA** *and* **.P?0** *files only* - **?** = **A** - **Z**).

The Save Button

The **Save** button is used to save the current workbench definition as an **.IOB** file. Saving the workbench definitions to an **.IOB** file is important if you want these definitions to persist between SIMION sessions.

If any array has been fast adjusted recently, you will be asked if you want to save it too. The only reason for saving these changes is if you plan to load it outside of an **.IOB** file (*e.g. with* **Old** *or* **Load**) and want the potentials conserved. ***Remember the .IOB contains the active potentials at the time of .IOB file saving, and SIMION can restore these potentials whenever the .IOB is loaded.***

Also, if the **Align** button is currently depressed, you will be asked if you want the workbench saved with the current alignment active.

Saving Kept Ion Trajectories with an .IOB File

If you have kept trajectories (*using Keep button*) when you save an **.IOB** file, SIMION will ask if you want to save an auto-loading **.KEPT_TRAJ** file too. If you want to delete the **.KEPT_TRAJ** file, use the GUI file manager. The **.KEPT_TRAJ** file will remain unchanged unless you choose to update it with the currently active kept trajectory images during an **.IOB** save.

Saving Ion Definitions with an .IOB File

When you save an **.IOB** file, SIMION will ask if you want to save the current ion definitions to an auto-loading ion definition file (*.**FLY** or .**ION** depending on what ion definitions you are currently using*). An auto-loading ion definition file has the same name as the **.IOB** file with a **.FLY** or **.ION** extension (*you can simply copy and/or rename ion definition files to make them auto-loading*).

Saving Data Recording Definitions with an .IOB File

When you save an **.IOB** file and data recording is active (***Record** button is depressed*), SIMION will ask if you want to save an auto-loading data recording definition file (*.**REC***). An auto-loading data recording definition file has the same name as the **.IOB** file with a **.REC** extension (*you can simply copy and/or rename data recording definition files to make them auto-loading*).

The Load Button

The **Load** button is used to load an **.IOB** file and its workbench definitions and make them the current workbench definitions for the **View** function. Any required potential arrays that are ***not*** already in memory will automatically be loaded. SIMION will ask if you want the array potentials ***restored*** to the values active when the **.IOB** was last saved/replaced. If you select **Yes** (*the default*) SIMION will automatically fast scale **.PA** files and fast adjust **.P?0** files to restore their potentials.

It is ***not*** recommended that you use the **Load** button to routinely load workbench definitions. The suggested method is to exit **View**, remove all PAs from RAM, and then re-enter **View** - forcing an automatic **.IOB** load request. ***This approach minimizes the clutter of PAs in RAM.***

Auto-loading Kept Ion Trajectories with an .IOB File

When SIMION loads an **.IOB** file it will automatically load any associated **.KEPT_TRAJ** file into a temp kept trajectory file for immediate viewing. If you want to delete the **.KEPT_TRAJ** file, use the GUI file manager.

Auto-loading Ion Definitions with an .IOB File

When SIMION loads an **.IOB** file it will automatically load any associated **.ION** or **.FLY** file as the currently active ion definitions (*with your permission*). If both an auto-loading **.ION** and **.FLY** file exists, SIMION will preferentially auto-load the **.ION** file.

Auto-loading Data Recording Definitions with an .IOB File

When SIMION loads an **.IOB** file it will automatically load (*with your permission*) any associated **.REC** file as the currently active data recording definitions, ***and automatically turn data recording ON (e.g. depress the Record button for you).***

Instance Alignment Beams

The **X**, **Y**, and **Z** buttons on the Normal Controls Screen activate x, y, and z axis instance alignment beams. The alignment beams pass through the working origin of each array instance and are aligned with their PA's x, y, or z axis respectively. Thus if two instances exist and the **X** alignment beam button is depressed ***two*** x-axis alignment beams will be drawn - ***one for each instance***.

Alignment beams are often useful for checking instance and ion beam positioning.

Hidden Line Drawing Controls

The **Hidden** and **Clip** buttons are used to control hidden line removal for ***alignment beams***, ***contours***, and ***ion trajectories*** (*only*).

The Hidden Button

When the **Hidden** button is depressed (*its default*) SIMION uses hidden line drawing methods to remove portions of alignment beams, contours, and ion trajectories that are visually blocked by instance images.

The Clip Button

The **Clip** button allows clipping control of ion trajectories, axis lines, and 3D contours in cutaway clipped 3D views. With the **Clip** button raised (*the default*), these vectors are only clipped at the outer 3D volume's boundary. This means that when you use cutaway clipping the ion trajectories, axis lines, and 3D contours will be drawn in the cutaway volume (*by default*). If you depress the **Clip** button these features will be fully clipped as they were in SIMION 6.0.

The Ion Flying Controls

The Normal Controls Screen also has a collection of ion flying controls. ***These controls are discussed in Chapter 8***.

The PA Instance Control Screen

The PA Instance Control Screen is used to add, delete, and edit instances of potential arrays (*Figure 7-20*). The control screen is accessed by clicking on the **PAs** tab or hitting the **P** button.

Instance Selection, Information, and Access Controls

The right two thirds of the PAs Control Screen contains controls to select an instance, display its PA's description, and access/control various items.

The Instance Selection Panel

The **Instance Selection** panel is used to display/select the currently selected instance. An instance must be selected ***before*** it can be acted on by operations like **edit** and **delete**. The currently selected instance is outlined by a green box and its x, y, and z axis are drawn to aid in visualizing its orientation.

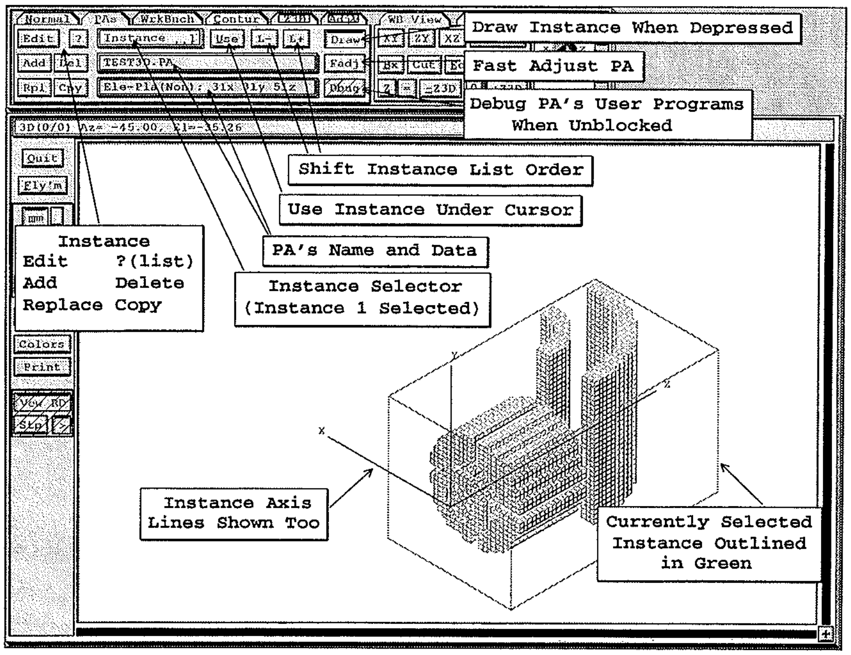


Figure 7-20 The PA instances control screen

The Use Button

The **Use** button is useful for quickly selecting an instance with the cursor in ***any*** WB View. Just point the cursor at the desired instance and hit the **U** key. SIMION will select the nearest instance to the cursor location as the currently selected instance and outline it in green.

The Down 1 Button

Moves the currently selected instance down one in the instance list towards ***lower*** priority *(e.g. was 2, now 1)*. ***Instances with lower priority are not as likely to be visible to ions.***

The UP 1 Button

Moves the currently selected instance up one in the instance list towards ***higher*** priority *(e.g. was 1, now 2)*. ***Instances with higher priority are more likely to be visible to ions.***

The PA Data Displays

Two display objects are provided to describe the potential array that is referenced by the currently selected instance. In Figure 7-20, the array's name is **TEST3D.PA** and it is an electrostatic planar non-mirrored 3D array with dimensions of : 31x, 31y, and 51z.

The Fadj Button

The **Fadj** button is used to access the fast adjust function for the array referenced by the currently selected instance. If the referenced PA is not fast adjustable and/or fast scaleable *(e.g.* **.PA#***)* access to the button will be blocked. Note: The actual PA *(memory copy)* is fast adjusted *(and/or fast scaled)*. ***If more than one instance references the same PA, any fast adjust changes in one of these instances will affect the others too!***

The Dbug Button

The **Dbug** button is provided to allow quick debug access to any user programs associated with the instance's potential array. This button is a direct link to the user program development system. Access to the button will be blocked if the potential array doesn't have any associated user programs (*e.g. a* **TEST.PRG** *file for a* **TEST.PA** *array file) or* ions are currently flying. ***See Appendix I for information on user programs.***

The Draw Button

The **Draw** button controls the drawing of the instance. If the button is depressed (*the default*) the instance will be drawn if and only if its associated **E** or **M** button ***is not*** depressed. If the **Draw** button ***is not*** depressed the instance ***will not*** be drawn.

Just because an instance is invisible to you, doesn't mean SIMION won't see it. ***Ions fly through and collide*** (*splat*) ***with invisible instances just as if they were visible.***

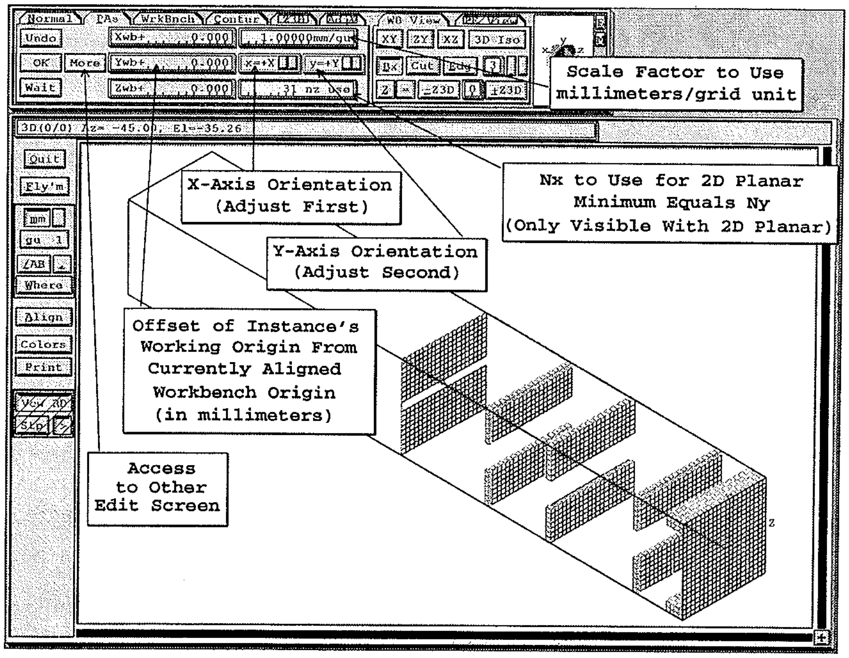


Figure 7-21 Primary instance parameter editing screen

The Edit Button

The **Edit** button is used to edit the positioning, scaling, and orientation of the currently selected array instance (**Instance Selection** *panel*). To edit an instance, select it with the **Instance Selection** panel and then click the **Edit** button. SIMION automatically switches to the first of two instance parameter editing screens (*Figure 7-21 above*).

The Undo Button

The **Undo** button is visible on ***both*** edit screens. It is used to restore the positioning, scaling, and orientation to what they were when the **Edit** button was ***last*** clicked.

The OK Button

The **OK** button is visible on ***both*** edit screens. Clicking the **OK** button accepts the changes and returns you to the PA Instance Control Screen. Unless the **Wait** button is depressed, switching to another control screen (*e.g. the Normal Controls Screen*) is the same as clicking the **OK** button (*any instance editing changes are kept*).

The Wait Button

The **Wait** button is visible on ***both*** edit screens. When it is depressed any editing changes are delayed until the **Wait** button is clicked again or the **OK** button is clicked.

Normally SIMION changes the instance interactively as you edit its parameters. This allows you to see the results of your editing immediately. The **Wait** button is provided to allow you to make several changes without creating a flurry of re-draws.

The Xwb, Ywb, and Zwb Panels

These three panel objects display/control the offset position of the instance's ***working origin*** from that of the ***currently aligned*** ***workbench origin***. The units of offset are millimeters.

The Scaling Panel

The **Scaling** panel displays/controls the scaling of the instance units (*gu*) into workbench units (*mm*) via the ***mm/gu*** scale factor. The default value is 1.0 millimeter/grid unit.

The Two Orientation Selectors

There are two **Orientation** selectors (*Figure 7-21 above*). These are used to display/control the instance's angular orientation. ***All*** angular rotations are made about the instance's ***working origin***. These selectors are coupled with the **Az**, **El**, and **Rt** panels on the secondary instance parameter editing screen (*accessed via the* **More** *button*).

Use the **Orientation** selectors to insure that the instance will be integrally aligned with the ***currently aligned*** ***workbench coordinates***. If the instance is not integrally aligned the **Orientation** Selectors will display *x= ?* and *y= ?*.

When adjusting the **Orientation** selectors, adjust the **x=** selector ***first*** and the **y=** selector ***second***. The **x=** selector allows six orientations (*+x, -x, +y, -y, +z, and -z*). The **y=** selector has four orientations that depend on the orientation of the **x=** selector.

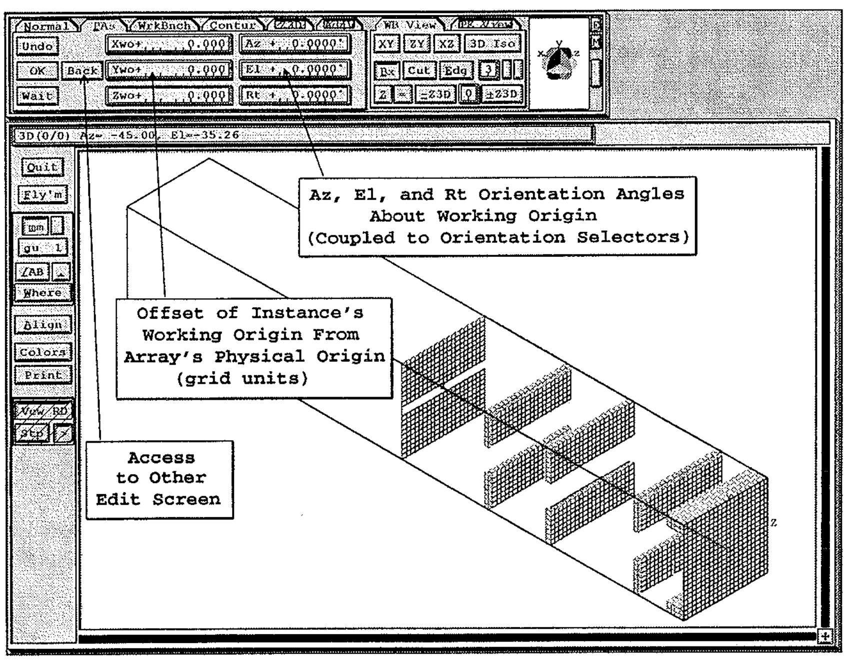


Figure 7-22 Secondary instance parameter editing screen

The More Button

The **More** Button is used to access the secondary instance parameter editing screen (*Figure 7-22 above*). This secondary instance parameter editing screen has controls to display/adjust the offset of the working origin from the array's physical origin and the azimuth, elevation, and rotation angles for orienting the instance in the ***currently aligned* workbench coordinates**.

The Back Button

The **Back** button is used to return to the primary instance parameter editing screen (*Figure 7-21 above*).

The Xwo, Ywo, and Zwo Panels

These three panels are used to display/control the offset of the instance's ***working origin*** from the ***physical origin*** of the potential array. The units of offset are potential array grid units. This offset is normally 0,0,0 – the instance's ***working origin*** is the array's ***physical origin***.

The Az, El, and Rt Panels

These three panels are used to display/control the orientation angles (*in degrees*) of the instance relative to the ***currently aligned* workbench coordinates** (*Figure 7-22 above*). A diagram of how these angles work is at the beginning of this chapter. ***These controls are normally used to define a non-integrally aligned orientation.***

The **Az**, **El**, and **Rt** controls are interconnected with the **Orientation** selectors on the primary instance parameter editing screen (*Figure 7-21 above*). In order for an instance to be integrally aligned with the ***currently aligned* workbench coordinates** each of these angles must be integrally divisible by 90.

The ? Button

If you click the '**?**' button on the PAs Options screen, the data monitor will appear and display all the parameters for the currently selected instance. If data recording is active, you can save this information to a file. The parameters for multiple instances can be recorded by selecting each desired instance in turn (*via the Instance Selection panel*) and then clicking the '**?**' button. If data recording is not active, the data monitor screen will disappear when you start the next Fly'm or exit and reenter View. ***See Chapter 8 for more information on data recording and the data monitoring screen.***

The Add Button

The **Add** button on the PA Instance Control Screen is used to add an instance to the workbench. The following procedure is used to add an instance:

1. Mark the volume you want the instance to be in. If you don't define a volume, SIMION will assume that you want the instance to fill the current workbench volume. ***You may want to increase the workbench size first (see Workbench Control Screen info. below).***
2. Click the **Add** button. SIMION will use the GUI File Manager to assist you in selecting the potential array to couple to the instance. Point to the desired potential array's button and click ***both*** mouse buttons (*only **refined** **.PA** and **.P?0** array files are useful for ion flying*). SIMION will automatically load the potential array if it ***is not*** already in RAM.
3. You will now see an instance edit screen that contains the parameters that SIMION plans to use for the instance (*Figure 7-23 below*). Edit the values of these parameters as desired. Now click the **Done** button and the instance will be added to the end of the list (*as highest numbered instance = highest priority*).

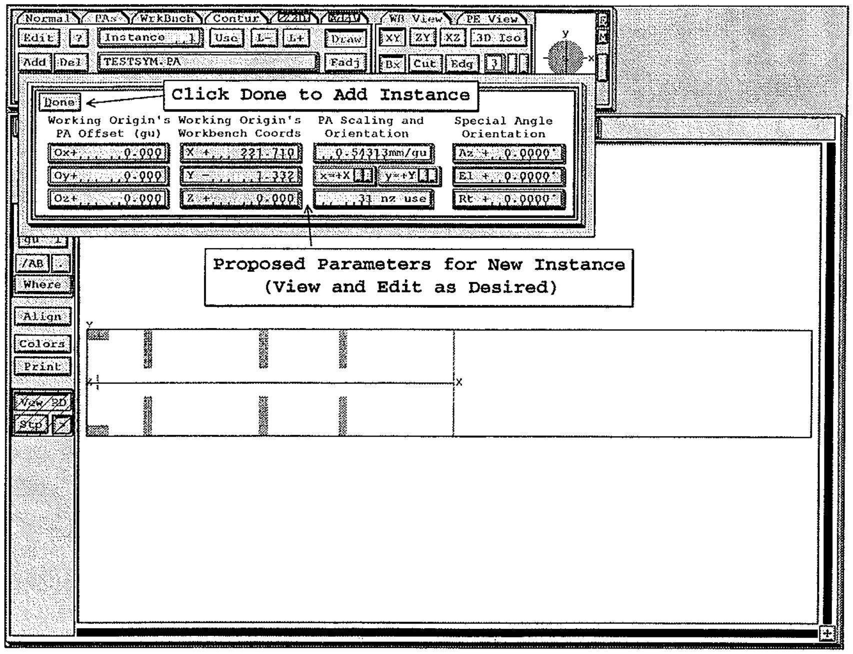


Figure 7-23 New instance parameter editing screen

You can then click the **Edit** button to edit the instance further as described above, use the **Up 1/Down 1** buttons to change the instance's priority order in the instance number list, or use the **Del** button to delete it (*assuming you really blew it*).

The Del Button

The **Del** button is used to delete the currently selected instance. To delete an instance, use the **Instance Selection** panel to select the desired instance. Click the **Del** button. SIMION will ask if you're sure. ***Click* Yes *and it's all over but the shouting*.**

The Rpl Button

The **Rpl** button is used to change the potential array that is referenced by an instance ***without*** changing ***any*** of the instance's positioning, scaling, and orientation parameters. Thus **Rpl** allows you to substitute one potential array for another. One could use **Rpl** to connect a **.PB0** array into an instance that formerly was connected to a **.PA0** array. This allows different instances to of the same array to have different potentials (*discussed previously*).

To replace an array, use the **Instance Selections** panel to select the desired instance. Click the **Rpl** button. SIMION will use the GUI File Manager to assist you in selecting the replacement array. Point to the array's button and click ***both*** mouse buttons.

The Cpy Button

The **Cpy** button provides a method to copy overlapping electrode (*or pole*) points from instances (*of the same type - e.g. electrostatic to electrostatic*) to the ***equivalent*** locations on the ***currently selected 3D (non-mirrored) potential array instance***. ***This is an advanced SIMION feature used to help model interactions between instances.***

For example, let's say we have a collection of instances inside a larger 3D potential array instance (*the can*). Let's also assume that the instances interact electrostatically (*e.g. it is not field-free between them*). What we need is a way to model the effects of the interior instances on the fields of the containing 3D potential array instance. ***We could do this if we could project the appropriate electrode points from the interior instances into their equivalent 3D array instance points***. We would then refine the 3D array to estimate the fields outside the interior instances.

For this problem, let's also assume that the 3D array is a **.PA0** fast adjust and that we want to be able to vary the effective voltages of the interior instance electrodes too. The first step would be to create the externally equivalent potential arrays for the internal instances. In most cases (*good design*) cylindrical potential arrays are enclosed by a tube. This means that the array looks like a solid tube to a outside observer. Thus one would use **Modify** to create a solid tube (*bar*) starting with the original array. If the tube is to be fast adjustable it should be given a potential appropriate to mesh properly with the 3D array's **.PA#** file and the file saved with a different name. Now load the desired **.IOB** file and use **Rpl** (*above*) to load the 3D **.PA#** file into ***its instance*** as well as the solid cylinder array into its appropriate instance. Now switch to the 3D instance, use the **Cpy** Button to copy the points from the solid cylinder. Now exit **View** and **Refine** the **.PA#** file. You can now get back into **View** and use **Rpl** to restore the original potential arrays to their proper instances (*be sure to save the .IOB file afterwards*).

Note: Because the destination 3D array is ***generally*** at much lower resolution than the source array you may have problems with ions splating on the crude array below as they exit the higher resolution array above (*in instance list order*). This problem can be avoided by slightly expanding the size of the interior potential arrays with an expanded boundary area (*volume*) of non-electrode points. This helps ions transition beyond any copied points (*and thus no splat*).

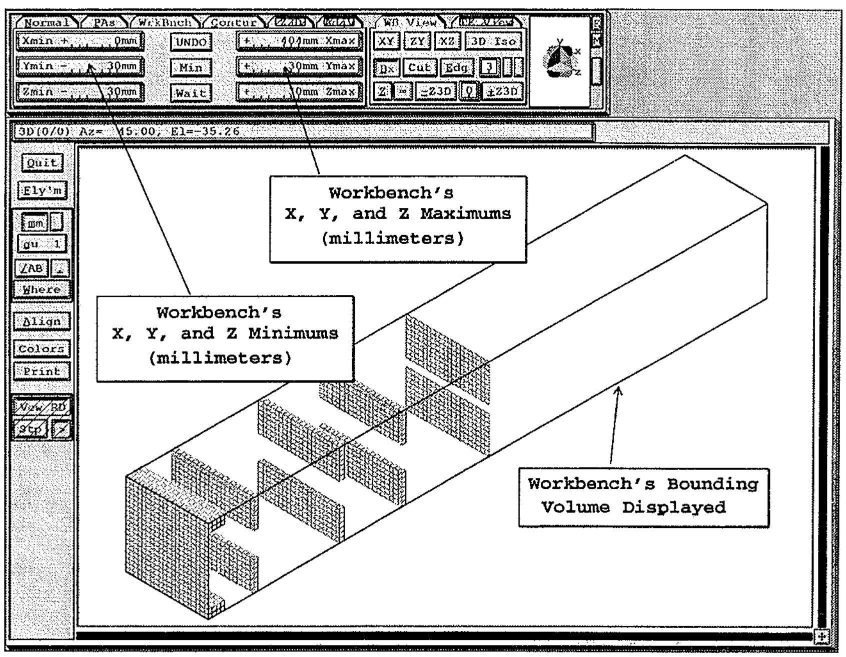


Figure 7-24 Workbench Control Screen

The Workbench Control Screen

The Workbench Control Screen is accessed by clicking the **WrkBnch** tab. This screen has objects that display/control the size of the current workbench (*Figure 7-24 above*).

The Undo Button

Clicking the **Undo** button restores the workbench size that was active when the Workbench Control Screen was entered (*when the* **WrkBnch** *tab was last clicked*).

The Min Button

Clicking the **Min** button reduces the size of the workbench to the ***minimum volume*** that the currently defined instances will just fit within.

The Wait Button

Normally SIMION changes the workbench volume interactively as you change the workbench volume parameters. However, if you depress the **Wait** button, SIMION will allow you to adjust the workbench dimension panels without immediately applying the changes to the workbench. ***Remember!*** You must click the **Wait** button (*to raise it*) ***before*** your modifications will be applied to the workbench.

The Xmin, Ymin, Zmin, Xmax, Ymax, and Zmax Panels

These six panel objects display/control the dimensions of the workbench in ***currently aligned workbench coordinates***. The units are in ***integral millimeters***. You ***will not be allowed*** to adjust the workbench to a volume that would be ***smaller*** than the volume required to contain the currently defined instances.

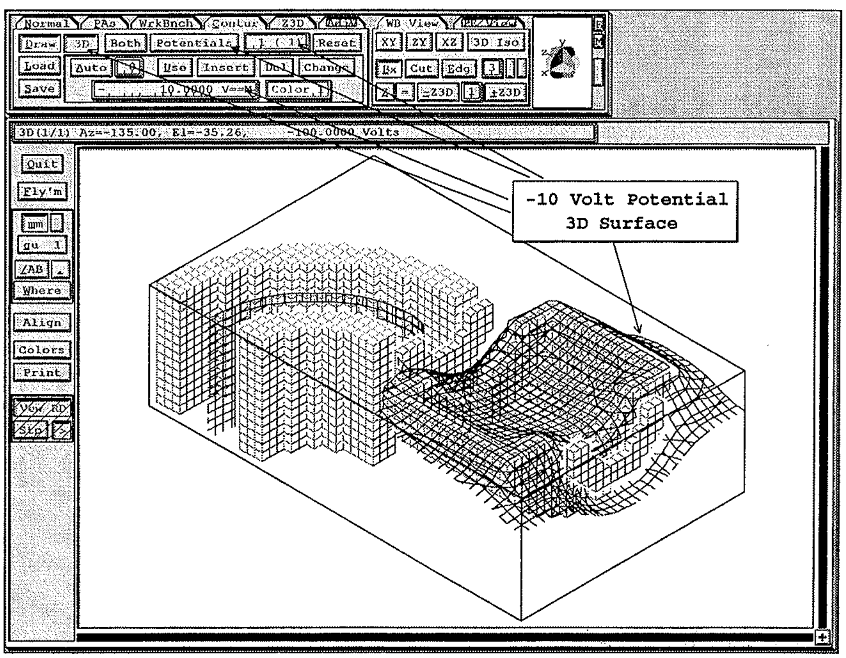


Figure 7-25 Example of a 3D contoured potential surface

The Contour Control Screen

Click the **Contur** tab or hit the **C** key to access the Contour Control Screen (*Figure 7-25 above*). The Contour Control Screen is used to control the drawing of potential and/or gradient contours as well as 3D contour surfaces.

Instances Must be Integrally Aligned

Contours will ***only*** be displayed for instances that are ***integrally aligned*** with the ***currently aligned* workbench coordinates**. You can integrally align any instance (*that is not currently integrally aligned*) by making it the currently selected instance via the **Instance Selection** panel on the PAs Control Screen (**PAs** *tab*), and then depressing the **Align** button.

Types of Contours

SIMION will draw potential (*volts or Mags*) ***and/or*** gradient (*volts/mm or Gauss*) contours of electrostatic and magnetic instances. Up to ***99*** contours of each type (*potential and gradient*) can be currently defined. Each contour is defined by its potential or gradient value and its color (*index*). ***Note: Contour colors are separately controllable.***

Contours can be drawn either as lines or 3D surfaces. Your contouring options depend on the view selected (*e.g. WB or PE*).

Contour Lines

Contour lines can be drawn in any WB or PE View.

Contour Lines in PE views

PE Views support the drawing of contour lines (*only*). The status of the **3D** button is ***ignored***. These contour lines are the same as shown in the equivalent ***standard angle 2D*** WB View.

Contour Lines in 2D WB Views

Contour lines are drawn ***standard angle 2D*** WB Views (*the* **Exact Angle** *button must be off*). The status of the **3D** button is ***ignored***. The instance must be drawn (*e.g. its* **Draw** *button depressed and its type button raised* - **E** *or* **M**) for ***standard angle 2D*** WB View contours to be drawn.

When SIMION displays contour lines in ***standard angle 2D*** WB Views, it is ***only*** displaying them for ***one layer*** of each integrally aligned instance that is visible within the current WB View volume. ***The question is, which layer?*** The following explains the layer selections rules (*same rules as for PE View surfaces*):

Rules for 2D and 3D Planar Instances

SIMION uses a simple layer selection rule for 2D and 3D Planar instances. Start inward from the front surface of the current WB View volume (*as currently displayed on the view screen*) and display the first instance layer encountered. An instance layer is just like a layer in the **Modify** function (*a **plane** of array points*). ***SIMION always uses the nearest plane of array points for its selected contour surface layer.***

This means you can see the contour lines of layers inside an instance by cutting inside it with a 3D Zoom.

Rules for 2D Cylindrical Instances

2D cylindrical instances present a special problem for contouring. What you normally want to contour is the ***on x-axis layer*** (*central plane view*) assuming you're ***not*** looking at the instance from an end-on view. ***When the view of a 2D cylindrical instance is not an end-on view, SIMION normally contours the central plane (x-axis layer) view.***

If you want to view other layers of the volume in a side view of a 2D cylindrical array, click the **Edg** button. SIMION now treats the 2D cylindrical array as if it were actually its pseudo-equivalent 3D Planar dual for layer selection and contour generation.

Contour Lines in 3D WB Views

Contour lines are drawn in ***standard or exact angle 3D isometric*** WB Views when the **3D** button (*on Contour Control Screen*) is ***not*** depressed ***or*** the **Edg** button ***is*** depressed. ***Contours of 3D WB views will be drawn whether the instance itself is drawn or not.***

The three visible boundary planes of the ***current volume*** (*workbench or 3D zoom*) are used for determining the layer of the instance used for contouring. The instance layers that are used for contouring are those layers that ***actually intersect*** one of the three visible boundary planes. ***If no instance layer intersects a visible boundary plane no contour lines from that instance will be drawn in that boundary plane.***

3D Contour Surfaces

3D Contour Surfaces are only drawn in ***standard or exact angle 3D isometric*** WB Views when the **3D** button (*on Contour Control Screen*) ***is*** depressed ***and*** the **Edg** button ***is not*** depressed. ***Contour surfaces of 3D WB views will be drawn whether the instance itself is drawn or not.*** Thus you can make an instance invisible and SIMION will ***still*** draw its 3D contour surface(s).

Unlike contour lines, 3D contour surfaces will be drawn for all instances that appear within the ***current volume*** (*workbench or 3D zoom*). Use the **Hidden** and **Clip** buttons on the Normal Controls Screen to control hidden line drawing for 3D contour surfaces.

Contouring Controls

The Contouring Control Screen contains a collection of control objects. Note: SIMION uses the current **Drawing Quality** panel's value (*0 lowest - 9 highest*) of the current view type (*WB or PE*) to determine the quality level to draw any contours. The following is a tour of these objects to help you understand how to use them.

The Draw Button

The **Draw** button forces the drawing of all contours (*if defined*) when ***depressed***. Once this button is depressed, contours will be drawn whenever the view is redrawn. To stop contour drawing click the **Draw** button to raise it.

Remember, if contouring is taking too long, you can always hit the **Esc** key to halt contour drawing on the current view (*seldom necessary*).

The Load and Save Buttons

SIMION allows you to save contour definitions to **.CON** files. The **Load** and **Save** buttons on the left edge of the Contour Control Screen are used to load and save **.CON** files (*via the GUI File Manager*). A contour file (*e.g.* **TEST.CON**) contains the definitions for all the potential ***and*** gradient contours defined when the file was last saved.

The Both Button

When the **Both** button ***is*** depressed, both the potential and gradient contours will be displayed. If the button to the right displays potentials, then the gradient contours will be drawn first (*if defined*) followed by the potential contours (*if defined*). Otherwise, the drawing order will be reversed.

When the **Both** button ***is not*** depressed only the contours of the currently selected type (*e.g. Potentials in Figure 7-25*) will be drawn.

The 3D Button

The **3D** button (*when depressed*) tells SIMION to draw 3D surface contours in ***standard and exact angle 3D*** WB views. If the **Edg** button is depressed the **3D** button status will be ignored. ***It is recommended that you not draw more than one 3D surface contour*** (*things can get pretty confusing*).

The **Hidden** and **Clip** buttons (*on the Normal Controls Screen*) can be used to control the hidden line removal drawing of the 3D surface contours. You may also want to suppress drawing of the instance itself to aid in viewing the 3D surface contours (*via the instance's* **Draw** *button or the* **E** *or* **M** *button*).

The Potentials / Gradients Button

To the right of the **Both** button is the **Potentials / Gradients** button. It is used to select the type of contours to be drawn, defined, and/or edited. Click this button to switch between contour types. Up to ***99*** contours of each type can be defined at the same time.

The Contour Selection Panel

Immediately to the right is the **Contour Selection** panel. It displays two numbers. The ***leftmost*** number is the currently selected contour number, and the ***rightmost*** number is the total number of currently defined contours of the selected contouring type (*potentials or gradients*).

SIMION automatically keeps all contours of the same type in a sorted list from 1 (*smallest value*) to n (*highest value*). When you use the panel to select a contour by its number, SIMION will automatically display its value and color in panels at the bottom of the control screen.

The Reset Button

The **Reset** button is used to reset (*erase*) all contour definitions of the currently selected contouring type (*potentials or gradients*). SIMION will ask if you are sure before erasing these contour definitions.

The Auto Button

The **Auto** button is used to automatically generate ***potential*** contours. Contour definitions will be generated using the ***currently selected instance*** (*PAs Control Screen via* **Instance Selection** *panel*). There are two types of automatic contours depending on the value of the **Automatic Contour Number** panel immediately to the right.

The normal procedure for automatically creating contours is to select the color desired for the automatic contours (*via the* **Color** *panel*), select the number and type of automatic contours (*via the* **Automatic Contour Number** *panel*), and then click the **Auto** button. SIMION will scan the currently selected instance, generate the list of potential contours (*replacing any that are currently defined*), and then depress the **Draw** button (*if required*) to force the new contours to be drawn.

The Automatic Contour Number Panel

This panel controls the number and type of automatic potential contours generated depending on its value.

A Value of Zero (0)

If this panel has the value of zero, SIMION will scan the currently selected instance for electrode/pole points and remember their potentials. It will then create contours at each of these potentials ***and*** at potentials 10% above and below these potentials to the next higher and lower potential. If the number of contours thus generated would exceed 99, SIMION will reduce the number of contours defined.

Values Greater Than Zero

If this panel has a value greater than zero (*e.g. 9*), SIMION will scan the currently selected instance for the range of electrode/pole potentials. It will then create the requested number of potential contours at equally spaced intervals ***between*** the maximum and minimum potentials found.

For example, if the maximum potential is 100 volts and the minimum is 0 volts, a panel value of 9 would result in contours being created at 10, 20, 30, 40, 50, 60, 70, 80, and 90 volts.

The Use Button

The **Use** button provides a second way to define contours. Switch to a ***standard angle 2D*** WB View, select the desired contouring type (*potentials or gradients*), set the desired color (**Color** *panel*), move the cursor to a point that the contour will cross, and hit the **U** key. SIMION will determine, insert, and draw (*if the* **Draw** *button is depressed*) the new contour. Its value and color will be displayed on the **Contour Value** panel and **Color** panel objects.

There is a second way to make use of the **Use** button. In this case you mark an area, and then click the **Use** button or hit the **U** key. SIMION will draw the contour through the ***center*** of the marked area.

The Insert Button

The **Insert** button provides a third way to define contours. Simply select the contour type (*potential or gradient*), enter its value in the **Contour Value** panel, enter its color in the **Color** panel, and then click the **Insert** button. If the **Draw** button is currently depressed the new contour will be drawn.

Note: SIMION will refuse to insert a contour that duplicates the ***value*** of any currently defined contour.

The Del Button

The **Del** button is used to delete contour definitions. There are two ways to make use of this feature. The first approach is to select the contour type (*potential or gradient*), select the desired contour using the **Contour Selection** panel, then click the **Del** button to delete it. If the **Draw** button is currently depressed the contour will be erased. ***This works in any view*** (*WB or PE*)

In the second approach use the mouse to mark the contour (*move the cursor to a location* ***on or near*** *the contour line then click the* ***left*** *button*). Now click the **Del** button to delete the selected contour. ***This only works in standard 2D WB Views.***

The Change Button

A contour's value and/or color can be changed via the **Change** button. Select the contour type (*potential or gradient*), select the desired contour using the **Contour Selection** panel (*the value and color will be displayed on the* **Contour Value** *panel and* **Color** *panel respectively*). Edit the contour's value and color as desired. Now click the **Change** button and the selected contour is changed. If the **Draw** button is currently depressed the contour will be redrawn as changed.

Note: SIMION will refuse to change a contour to a ***value*** that duplicates any other currently defined contour.

The Contour Value Panel

The **Contour Value** Panel displays the value (*potential or gradient*) of the contour currently designated by the **Contour Selection** panel. ***This is merely a copy of the contour's value.*** If you change it's value, nothing will happen until you click either the **Insert** or **Change** buttons.

The Color Panel

The **Color** panel displays the color of the contour currently designated by the **Contour Selection** panel. ***This is merely a copy of the contour's color.*** If you change it's color, nothing will happen until you click either the **Insert** or **Change** buttons.

The 3D Zoom Volume Control Screen

The 3D Zoom Volume Control Screen is used to control the size of a 3D zoom volume. To access this screen you ***must*** currently be 3D zoomed (*level 1 or higher*). Select the 3D zoom level to access and click the **Z3D** tab. SIMION will automatically ***delete*** any inner 3D zooms and display the 3D Zoom Volume Control Screen (*Figure 7-26 below*).

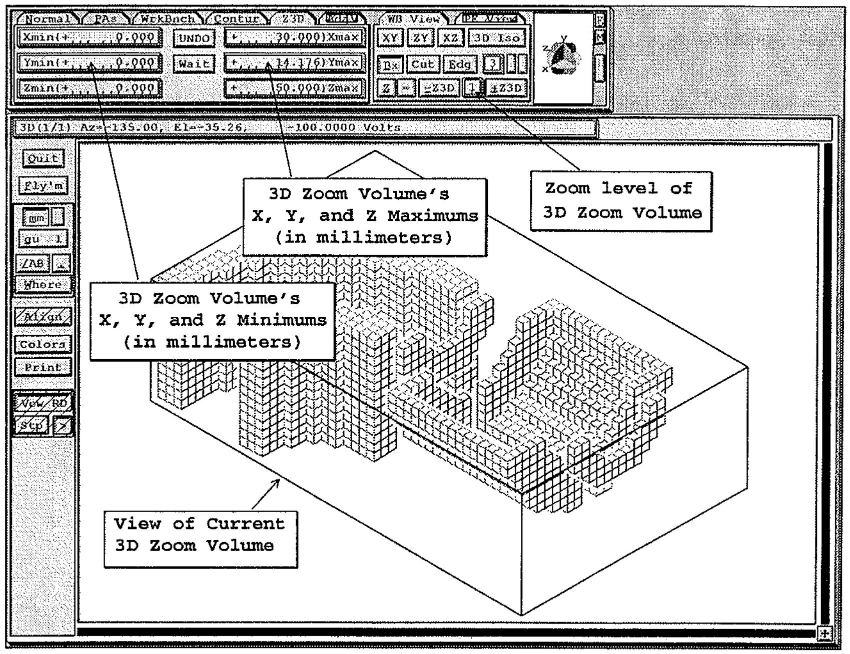


Figure 7-26 The 3D Zoom Volume Control Screen

The 3D Zoom Volume Control Screen allows you to set the exact size of the 3D zoom volume. This can be done while ions are flying. The feature is very useful for seeing how moving a plane of the current volume changes the contours or potential energy surfaces. ***You can, in effect, sweep through the 3D zoom volume.***

The UNDO Button

The **UNDO** button is used to restore the size of the selected 3D zoom volume to what it was before the **Z3D** tab was clicked to enter the 3D Zoom Volume Control Screen. ***Note:*** The **UNDO** button ***will not restore*** any lower level 3D zooms deleted when the **Z3D** tab was clicked.

The Wait Button

SIMION normally adjusts the 3D zoom volume interactively as you change any of its dimensions. However, there may be times when you want SIMION to wait. Depress the **Wait** button and SIMION will not make any changes in the 3D zoom volume until you click the **Wait** button again to raise it.

The Xmin, Ymin, Zmin, Xmax, Ymax, and Zmax Panels

These panel objects are used to display/change the current 3D zoom volume dimensions (*in millimeters*). The panel objects will not let you do anything illegal (*like negative size or a larger size than the next outer volume - workbench or 3D zoom volume*).

To change a dimension, select the appropriate panel and change its value. SIMION will re-size and re-draw the view as you change the panel's value. If you want SIMION to wait, depress the **Wait** button, make your changes, and then click the **Wait** button again (*to raise it*).

The Adjustable Variables Control Screen

The **AdjV** tab is used to access the Adjustable Variables Control Screen (*Figure 7-27 below*). This tab is normally blocked ***unless*** ions are flying with user programs active that have adjustable variables defined.

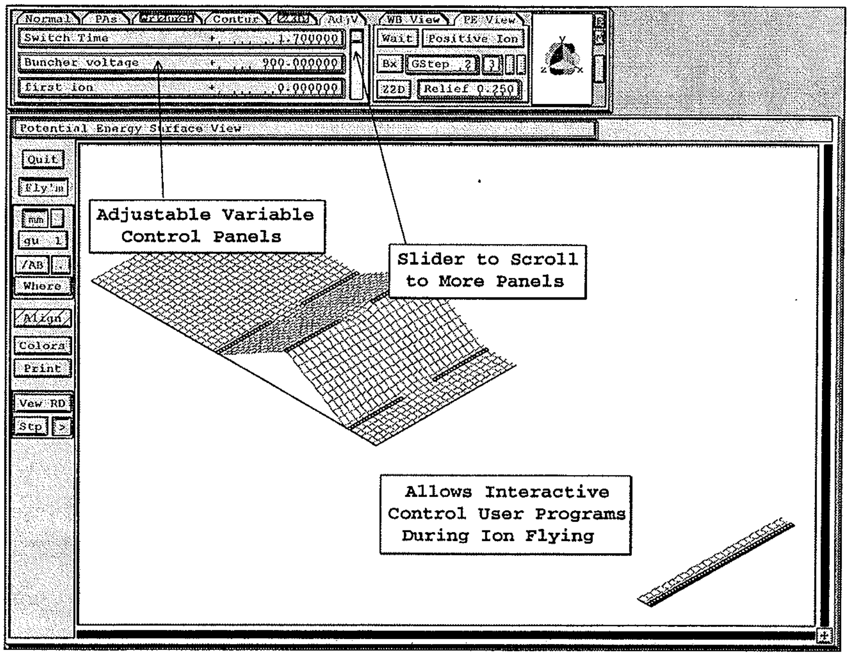


Figure 7-27 Adjustable Variables Control Screen (*User Programs*)

When you have user programs active that have adjustable variables defined, you can use this screen to change the values of these adjustable variables while the ions are flying. This is a useful feature if you want to adjust frequency, damping, or a wide range of other useful parameters.

Each adjustable variable has its own control panel with its name and value. A slider is provided to allow access to the list of adjustable variables - three at a time.

This control screen is discussed further in Chapter 8 and Appendix I.