Creating, Loading, and Saving Potential Arrays

Introduction

It is assumed that you have read the discussion of potential arrays in Chapter 2. If not, read the material before proceeding further. This chapter covers the creation of new potential arrays as well as how to save and load disk copies of potential arrays. Chapter 5 covers defining electrode/pole geometry via the Modify function. Chapter 6 covers the types of potential arrays and how they are created, refined, and fast adjusted.

The Role of the Subdirectory in SIMION Projects

SIMION requires that all files relating to a project (e.g. *.PA, *.IOB, *.FLY and etc.) are contained in the same subdirectory of your hard disk. This is useful because it keeps things together and in so doing forces a touch of organization that many of us need so badly. Note: There can be more than one project in a subdirectory. However, this can often contribute to a lot of clutter.

Each of the demos provided with SIMION is in its own directory below **\SIM7**. These demos help show how various projects might be approached.

The GUI File Manager can be used to quickly create subdirectories. To access the GUI File Manager click the **GUI File Manager** button on SIMION's Main Menu Screen. ***Click on the desired drive letter, click the desired parent directory, click the*** **Other** ***Button, enter the name of the new subdirectory in the Insert Directory ioline, and press*** **Enter**. The subdirectory is created. Now click on this subdirectory to make it the currently active directory. ***Note: The GUI File Manager can also be used to quickly copy or move files between directories and drives (see Appendix F).***

Working Copies of Potential Arrays are in RAM

SIMION maintains a working copy of each active potential array (*up to 200*) in memory (*RAM*). ***When you change something in a potential array you are only changing the in-memory copy.*** Likewise when you fly ions through array instances of potential arrays in the workbench volume you are using the in-memory array copies.

Copies of these in-memory potential arrays are normally saved as **.PA**, **.PA#**, or **.PA0** (*extension*) files in your project directory. When you create a new potential array ***only the in-memory copy is created***. It is your responsibility to save any new or changed potential arrays into your project directory as required. ***Saving potential arrays preserves your work between sessions***.

The List of Potential Arrays

The Main Menu Screen contains a window with a button for each currently allocated PA memory region and the name of its potential array (*Figure 4-1 below*). One of these buttons will be depressed indicating the array that is the ***currently selected potential array***. This is the array that will be acted upon by functions like: **Load**, **Save**, and etc.

A particular potential array is selected by clicking (depressing) its button.

There is a **PA's Require** panel at the top of the file list window that displays the number of megabytes of RAM currently allocated to potential arrays. This allocation includes the potential arrays in the list as well as any specific electrode solution arrays ***invisibly*** loaded to directly support fast adjust electrodes changed by any active **Fast_Adjust** user program segments (*Appendix I*).

The last button in the list is ***always*** marked **Empty PA**. The **Empty PA** is available for allocating memory for a new potential array. ***Up to 200 potential arrays can be loaded in RAM at one time (memory permitting).***

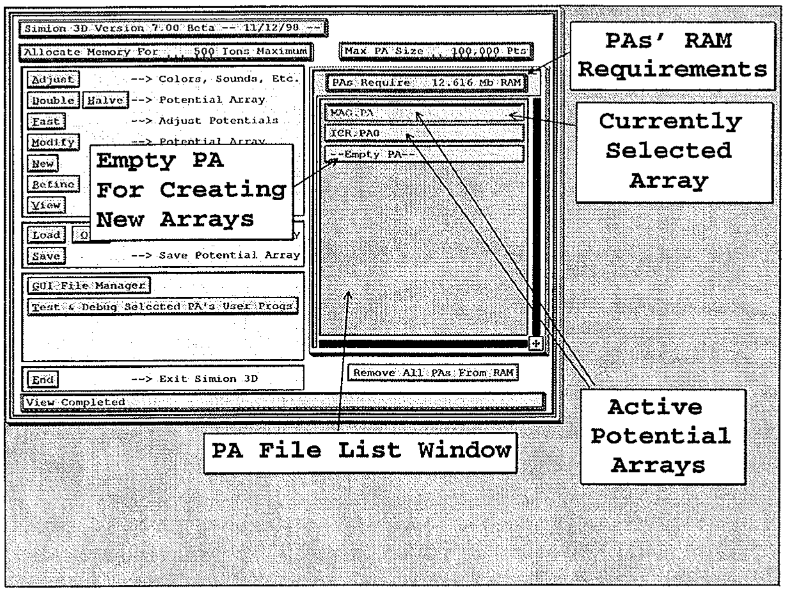

Figure 4-1 Potential Array File List Window

De-allocating Potential Array Memory

The Main Menu Screen has a **Remove All PAs From RAM** button (*Figure 4-1*). This button is used to remove all working copies of PAs from RAM. Its primary function is to restore a clean slate when you are about to start a new project or the clutter of PAs has become unmanageable. It is also useful to reduce heap fragmentation (*allowing larger blocks of RAM to be available for array allocation*).

It is possible that the above heap defragmentation approach may not always work because the operating system doesn't always consolidate returned RAM properly (*thank Bill*). This will manifest itself in a refusal to allocate array space that you know it should be able to. The only recourse is to save your files, exit SIMION, and then restart.

Memory Allocation for Potential Arrays

Potential arrays can use up a lot of memory. Each point of a potential array requires 10 bytes of RAM storage. Thus a 100 x by 100 y by 100 z 3D array has 1,000,000 points and requires 10 megabytes of RAM. ***SIMION allocates memory only once for each PA memory region it creates. Once a PA memory region has been allocated it is not returned or changed until the*** **Remove All PAs from RAM** ***button is used to remove all memory allocated to PAs (de fragment the heap).*** This is done to prevent heap fragmentation lockups due to the large size of typical potential arrays.

Changing the Default PA Memory Allocation

SIMION normally allocates a minimum of 100,000 points of memory (*1 MB of RAM*) for each new potential array. This is usually large enough to allow you to increase the array size (*e.g. via the* **Modify** *or* **Double** *functions*) without exceeding the memory allocated for a potential array. ***You have the option of adjusting this default PA memory allocation size up or down to suit your needs (with the* Max PA Size *panel object – Figure 4-1) before you create or load a potential array in an empty PA memory region (memory region size range: 20,000 to 50,000,000 points).***

Specifying Default Memory Allocation at Start-up

You also have the option of specifying the initial default memory to allocate for each new potential array at start-up. This is done by including the desired initial default allocation size in points on the SIMION command line (*e.g. found via the properties option in your Windows shortcut to SIMION*):

SIMION 0	Sets default to 20,000 points (*min. allowed*)
SIMION 1000000	Sets default to 1,000,000 points
SIMION 100000000	Sets default to 50,000,000 points (*max. allowed*)

How to Minimize RAM Usage

Use the minimum of 20,000 points for default PA memory allocation. This minimizes the amount of RAM required for ion optics bench definitions that involve many small potential arrays.

How to Increase a PA's Memory Allocation Region

You may on occasion need to expand a potential array's memory allocation region beyond its current *fixed* value (*e.g. to double it*). The following procedure can be used to accomplish this:

1. Save the potential array (*and any others you wish to keep*) to the current project directory.
2. Click the **Remove All PAs From RAM** button to de-allocate ***all*** potential arrays.
3. Adjust the **Max PA Size** panel to the desired memory to allocate.
4. Re-load the potential array into the **Empty PA**.

Creating New Potential Arrays

New potential arrays can be created either via the **New** function or by loading an existing potential array and saving it with a new name. In either case, the **Modify** function (*Chapter 5*) can ***then*** be used to redefine the new potential array and its electrode/pole geometry. ***Remember to save (replace) potential arrays after modifying them if you want changes to persist between SIMION sessions.***

Creating a Potential Array From an Existing Potential Array File

You can always use an existing potential array file as the start for a new potential array. The following procedure is recommended:

1. Click the **Empty PA** button on the Main Menu Screen if it is not already depressed.
2. Adjust the **Max PA Size** panel for a memory region of sufficient size for any planned array expansion.

3. Use the **Load** function on the Main Menu Screen to load an existing potential array into the **Empty PA** region.
4. Use the **Modify** function (*Chapter 5*) to re-define the potential array as required (*re-size and/or re-define electrode/pole geometry*).
5. Use the **Save** function to save a copy of the new potential array with its new name in the desired project directory.

Creating a Potential Array Using the New Function

The **New** function can be used to create a potential array. The following is the recommended

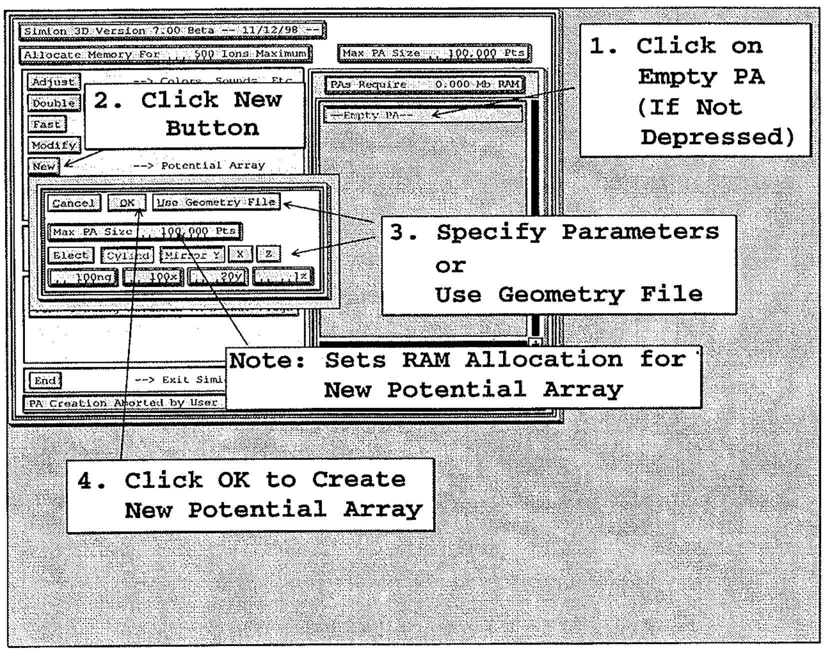

Figure 4-2 Creating a new potential array with the New Function

procedure (*see Figure 4-2 above*):

1. Click the **Empty PA** button on the Main Menu Screen if it is not already depressed.
2. Click the **New** button or press the **<n>** key to access the **New** function.
3. Specify the desired array parameters ***or*** click the **Use Geometry File** button (*advanced feature – Appendix J*). Note: The only important parameter is the array's RAM allocation (**Max PA Size** *panel*). ***All the other parameters can be changed later in the*** **Modify** ***Function.***
4. Click the **OK** button to create the new potential array.

Adjusting the Default Allocation Size within New

The **Max PA Size** panel (*in the New Function Screen*) defines the amount of RAM to allocate for the new potential array. The initial value will be the currently active default allocation value on the **Max PA Size** panel on the Main Menu Screen (*normally 100,000 points or 1 MB of RAM*). ***Any changes you make in allocation size will only impact RAM allocation for the new array***. The current default PA allocation will remain unchanged.

Be sure to allocate enough memory for any planned array expansion (*e.g. doubling*).

Adjusting Array Dimensions

The **x**, **y**, and **z** panels are used to specify array dimensions. Note: 2D arrays are specified when z = 1. 3D arrays are specified when z > 1.

The x, y, and z array dimension panels will not allow any array dimensions that would exceed the current maximum PA size. Thus, if you need a larger array, adjust the **Max PA Size** panel ***first***, then enter the desired array dimensions.

Selecting Electrostatic or Magnetic Potential Arrays

SIMION ***always assumes*** that you want an ***electrostatic*** potential array. If the array is to be magnetic, click the **Elect** button (*the title will switch to* ***Magnt***).

When a magnetic potential array is selected access to the **ng** panel will be unblocked. The default ng value is 100 (*details in Chapter 2*). You should set ng to the number of grid units of pole gap so that the magnetic potentials (*Mags*) are reasonably direct indications of the magnetic field in gauss between the pole pieces. ***The*** **ng** ***parameter can be changed later in the*** **Modify** ***function (Chapter 5).***

Cylindrical or Planar Symmetry

SIMION allows 2D arrays to have either planar or cylindrical (*volume of revolution*) symmetry. ***All 3D arrays must be planar (SIMION enforced).*** The **New** function assumes cylindrical by default. If you want planar click the **Cylind** button. ***Symmetry can be changed later in the*** **Modify** ***function (Chapter 5).***

Mirroring Options

You have the option of mirroring the potential array for negative x, y, and z array grid unit values. ***Mirroring can be changed later in the*** **Modify** ***function (Chapter 5).*** This can be used to reduce array sizes if the design symmetries allow. The **New** function assumes y mirroring by default. You can select what you desire. If the combination is illegal, SIMION will beep and restore the button to its former status. The possible array mirroring combinations are: **None, X, Y, Z, XY, YZ, XZ, XZY**. The legal mirroring combinations by array type are:

All 3D arrays:	All mirroring options are legal
Planar 2D arrays:	All mirroring except z are legal
Cylindrical 2D arrays:	***y mirroring*** is ***required***, x is legal, z is illegal

Using Geometry Files

You can also use geometry files to create new potential arrays. Geometry files are an advanced SIMION feature (*see Appendix J*). If the geometry file's first instruction is **PA_Define,** SIMION will use it to define the new potential array. Otherwise, SIMION will ask you if you want to use the array parameters defined on the New Menu Screen to create the potential array.

When you make use of geometry files within the **New** function SIMION will automatically insert the electrode/pole geometry defined in the selected geometry file into the newly created potential array. For a quick painless example of geometry files:

1. Click the **New** button on the Main Menu Screen (***Empty PA*** *button must be depressed*).

2. Click the **Use Geometry File** button.
3. You are now in the GUI File Manager. Click the **GEOMETRY** directory (*just below the* **\SIM7** *main directory*). Now point to the **TRAP1.GEM** button and click ***both*** mouse buttons to load and execute this file. An alternate method would be to click the **TRAP1.GEM** button and then the **OK** button.
4. Click the **View** button to take a look. This geometry file creates a simple 2D cylindrical symmetry hyperbolic trap.

Saving Potential Array Files

Potential Arrays in memory are saved to disk in the following manner (*Figure 4-3 above*):

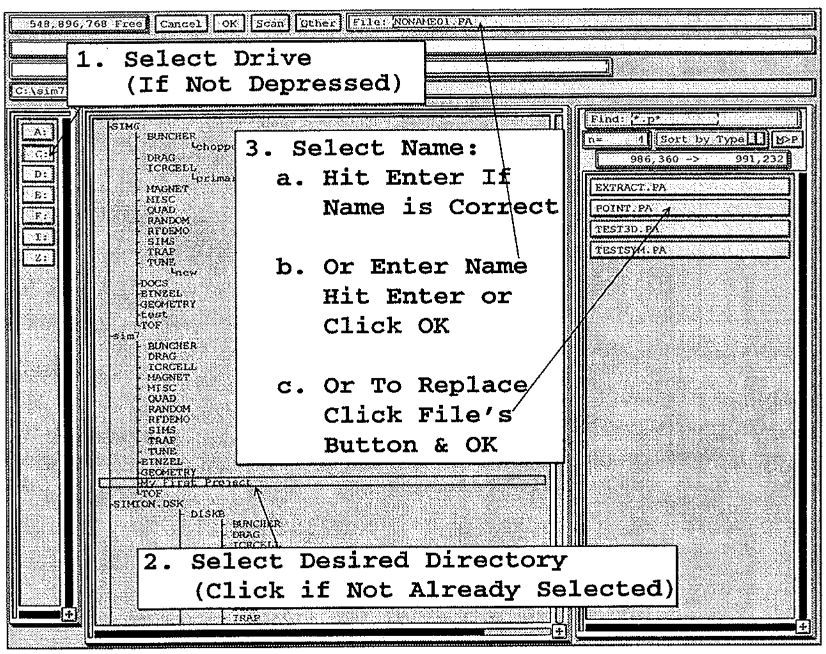

Figure 4-3 Saving a potential array using the Save function

1. Select the desired potential array to save by clicking its PA button (*if it is not already depressed*).
2. Click the **Save** button or hit the <s> key from the Main Menu Screen.
3. Select the destination drive and directory (*by clicking on them - if not already selected*).
4. Enter the desired file name and press **<Enter>** or click both mouse buttons on an existing file to replace it. ***Note: Long file naming conventions can be used*** (*e.g.* ***My First.pa#***)
5. If the name selected is that of an existing file, SIMION will ask if you want to replace it.
6. After the potential array is saved/replaced SIMION will display the file's current memo string for entry/editing (*Appendix F*). Press **<Enter>** if you want to skip memo entry/editing.

Legal File Extensions

SIMION generally allows only **.PA** (*Basic potential arrays*) and **.PA#** (*Fast Adjust Definition arrays*) to be saved by the user to disk. The other types of potential arrays are normally only created and saved by SIMION itself. This helps to prevent you from mucking things up accidentally. ***There are a couple of fast adjust file (.PA0) exceptions as listed below***:

Creating Secondary Fast Adjust Files (*e.g. .PB0*)

There are times when you may want two or more array instances of the same fast adjust array (**.PA0**) in the workbench with each instance ***having different voltages***. To avoid having to create and refine two or more identical **.PA#** arrays SIMION allows saving multiple **.PA0** files. This is accomplished by loading the desired **.PA0** file and then saving it as a **.PB0** file (**.PC0 - .PZ0** *are also legal to allow several such instances*). As long as the filename (*as opposed to its extension*) remains the same, SIMION will automatically use the same specific electrode solution files when fast adjusting each **.P?0** (*where ? is* **A-Z**) file.

Fast Adjust Files (*.PA0, .PB0, and etc.*)

SIMION will also allow you to ***replace*** (*via saving*) ***existing*** fast adjust **.P?0** files (*where ? is* **A-Z**) to retain the current adjustable electrode/pole potential settings between sessions.

File Memos

SIMION also allows you to attach a memo string to any file via its file manager (*see Appendix F*). This is often handy for including descriptions with your files (*even though long file names are supported in SIMION 7.0*). When you are in the GUI File Manager, a file's memo (*if any*) will automatically be displayed when you point the cursor to the file's button.

A file's memo can be edited from within the GUI File Manager by pointing to the file's button and then moving the cursor to the left off the button. This will retain the file's memo on the memo ioline object (*file's **short** name appears in the memo ioline to confirm selection*). You may now edit/create the file's memo. If you want help, point to the memo ioline object and hit the **<F1>** key for help.

File memos are kept in the **MEMOINFO.GUI** file in the ***same*** directory. Erasing this file erases all memos for files in the directory. ***The GUI File Manager will automatically copy/move the appropriate file memos when selected files are copied/moved via the file manager.***

Loading Potential Array Files into PA Memory

Potential array files on disk are loaded into PA memory in the following manner (*Figure 4-4 below*):

1. Select an existing memory region (*in-memory PA*) or **Empty PA** by clicking on its button.
2. Click the **Load** or **Old** button or hit the **<l>** or **<o>** key from the Main Menu Screen.
3. Select the source drive and directory (*if not already selected*).
4. Enter the desired file name and press **<Enter>** or click ***both*** mouse buttons on an existing potential array file's button to load it (*or click the file's name button and then click OK*).

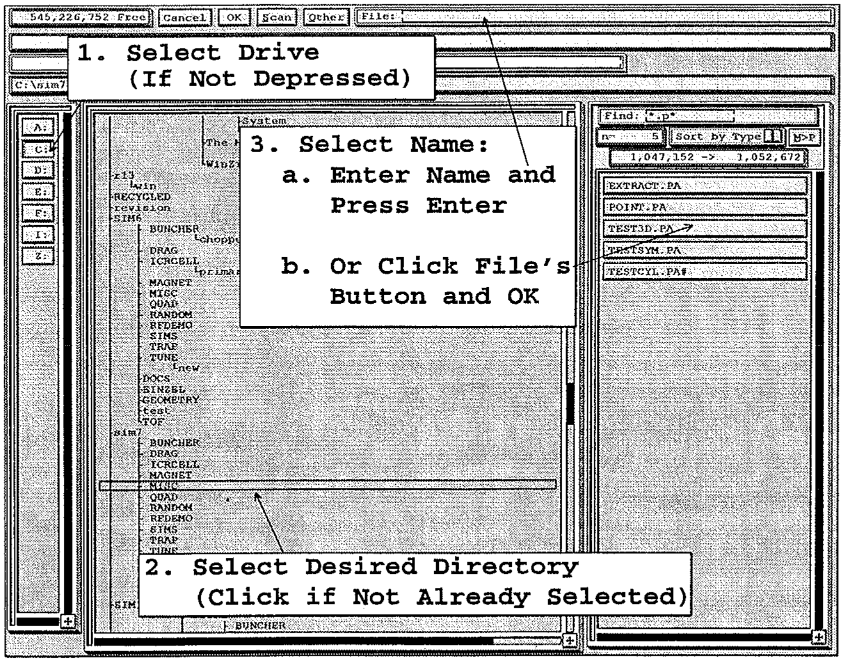

Figure 4-4 Loading a potential array into SIMION via the Old or Load function

Memory Allocation and Potential Array File Loading

If you select a non-empty PA (an existing PA), the PA file to be loaded cannot be larger than the size of its memory region. If you point the cursor at the PA's button (*on SIMION's Main Menu Screen*), the status line (*bottom object*) will display the PA's description along with the memory allocation for the region in points (*16356/100000 means: Current PA uses 16,356 points of 100,000 allocated to memory region*). ***SIMION will refuse to load any PA into a memory region that is not large enough to contain it.***

If you select the **Empty PA** button, SIMION will allocate the ***largest*** of either the current default region size (*the value of the* **Max PA Size** *panel*) or the actual region size required to hold the file. Thus if you load a million point PA file into the **Empty PA** when the **Max PA Size** panel is set to 100,000, the memory region allocated will be 1,000,000 points (*10 MB*), ***exactly*** enough for the PA file. ***If you plan to expand the size of the potential array later be sure the* Max PA Size *value is set high enough to allow for this planned expansion.***

Converting SIMION 2.0-5.0 Version Potential Arrays to SIMION 7.0 Format

SIMION 7.0 potential array files have a different format than versions of SIMION prior to 6.0. If you attempt to load a SIMION version 2.0 - 5.0 PA file, SIMION will ask you if you want it converted. If you say yes the existing file will be loaded ***and immediately re-saved*** as a SIMION 7.0/6.0 file. ***Thus you should hide from SIMION 7.0, any PA files that you don't want accidentally converted.***

Out of Heap Space Errors When Loading a Potential Array

SIMION will try to use existing RAM when loading potential arrays. However, when this is exhausted, SIMION will try to use virtual memory (*use disk for RAM*). If you are using SIMION 7.0 on Windows NT, an out of heap error ***probably*** indicates you need to expand your virtual memory size (*see Appendix B*). If you are running Window 95, you are probably out of disk space for your virtual memory scratch file.

Potential Array File Structure

See Appendix D for information on SIMION's potential array file structure. ***You may use this information to create or read SIMION 7.0 potential arrays with your own C programs.***

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