MacAtoms is a program for viewing atomic structures. The program gives you complete control over the parameters that determine the appearance of the picture. For example, you can change the viewpoint by just moving the mouse and observing the effect. Using the same technique, you can also change the radius of any type of atom, or the color used to represent it. You can also use the mouse to select a subset of atoms to be moved, to group atoms into molecules, or to cut and paste groups of atoms between windows.

The program places no limits on the number of atom types or the number of atoms of each type, beyond the obvious limitations imposed by memory. For many situations MacAtoms only requires 512K of memory, but you will find that you need more memory to display larger atoms, more complex images, etc. You will also need to increase the memory if you are going to do any printing.

Before you use MacAtoms, you must first prepare a data file that defines the atoms that are to be plotted. A simple example is shown below; you will find a detailed specification of the file in the user's manual. Prepare the file with any text editor that can save the file in "text only" mode; or prepare it on a mainframe and then upload it to your Macintosh. Once you have prepared the file, use the Open menu item; MacAtoms will then read commands and interpret them without further intervention on your part. This allows you to make movies while leaving the Macintosh unattended. To interrupt the process, insert a pause command in the file, or type a command-period. To have MacAtoms resume reading the file, select the Go item under the Action menu. Alternatively, press the return key.

To change a plot, decide what it is you want to change -- the viewpoint, the viewing distance, the radius of an atom, etc. Then select that thing from the Tools menu. For example, if you want to get a closer view, choose the item labeled Zoom. The cursor will change to a small magnifying glass indicates that you are in zoom mode. To change the thing you selected, just press the mouse button and move the mouse. You can use the command key shortcuts to select menu items more quickly. For example, command-Z will put you into zoom mode. Or, you can hold down a single key (without the command key) while you move the mouse. For example, holding down the Z key while you move the mouse will put you into zoom mode for as long as the key is held down.

When the Select One or Select Many tools are in effect, the mouse is used to select a group of atoms to be changed. To use the Select One tool, point at an atom and then click on it. To use the Select Many tool, press the mouse button and then drag the mouse from one place to another. As you do this, a rectangle will be drawn on the screen. When you release the mouse button, all the atoms within that rectangle will be selected. Selections may be grouped together to form molecules, and these groups may be combined to make other groups. Groups are formed by selecting some molecules and using the Group command on the Action menu. Thereafter, when one atom of a group is selected, all atoms in that group will be selected. Atoms may also

be assigned to groups in the data file.

While MacAtoms is at its best on those Macintoshes that can display gray scales and/or color, the program can also generate pictures on "one-bit" Macintoshes such as the Macintosh Classic, the SE, and many of the PowerBooks. To generate pictures on a one-bit Macintosh, MacAtoms uses a technique known as dithering. Although the program offers a choice of two dithering methods, the Peano curve algorithm is always the best. You will probably not need to use dithering on Macintoshes that support gray scale or color.

MacAtoms can produce hardcopy prints on any printer, including color as well as black and white printers and PostScript as well as non-PostScript printers. You can choose one of two printing methods by selecting the Print Method command from the File menu. The standard method works on all printers. The custom method is sometimes substantially faster than the standard method, but it works only on PostScript printers. MacAtoms can also drive several other types of recording devices besides printers -- for example, video tape recorders and optical disks.

If you are running System 7 or later, you can get more information about how to run MacAtoms by turning on Balloon Help.

Here is an example of a data file that specifies the unit cell for a body centered cubic crystal. To use this example, just copy the following lines into a text file, then open the file from MacAtoms. An easy way to do this is to select everything between the line above and one below using the mouse. (You may include these sentences if you wish; they will serve as comments in the data file.) Then use the copy command from the edit menu. Next start your favorite text editor or word processor and paste the text into a new file. Save the file as a "text only" file if your word processor gives you a choice. Finally open the new file from MacAtoms.

```
*atomdefs
2
20    65535        0    0
20        0    16367    0
*atoms
9
-75 -75 -75   1
-75   75 -75   1
 75 -75 -75   1
 75   75 -75   1
 0    0    0    2
-75 -75   75   1
-75   75   75   1
 75 -75   75   1
```

```
 75  75  75  1
*pause
```

Known problems:

You cannot use the control panel to change the number of shades of gray while running MacAtoms.

If two atoms are closer than the sum of their radii, the region of their intersection will not be plotted correctly. This is an unavoidable side-effect of the algorithm used to generate the pictures, which was chosen for its speed rather than its realism.

PICT images are not supported and probably will be dropped in future versions of the program.

If you allow MacAtoms to overlay pictures from two or more sets of atom coordinates, only the last set will be printed. This could be called a feature.

With System 6.0.4 and earlier, the colors are not changed properly when switching between applications. Also, the screen glitches when you change colors.

This version of MacAtoms is being offered as "Freeware", which means you don't have to pay me for it if you don't want to. However, the program is not in the public domain, and I retain all rights to it. Please distribute MacAtoms to your friends and to bulletin board systems, but do not modify the program or its messages in any way, and please _always_ include the documentation and sample data files with the program! You may give MacAtoms to your friends and include it in not-for-profit shareware distributions, but you may not sell it or include it as part of some other commercial offering without first signing a contract with me. If you didn't receive your version of MacAtoms directly from me, please drop me a postcard with your name and address. I would like to know which version of the program you have, how you got it, and how you intend to use it. In return I will keep you informed when new versions come out. If you need further information, wish to report bugs, or wish to make suggestions, please contact me at one of the places listed below. Note that I developed MacAtoms on my own time, so Sandia has nothing concrete to do with my mistakes.

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