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A Computer Graphics Program for Displaying Water Molecules on a DN3500 Apollo Workstation

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A COMPUTER GRAPHICS PROGRAM FOR DISPLAYING WATER MOLECULES ON A DN3500 APOLLO WORKSTATION*

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Abstract

A computer graphics program is developed for displaying water molecule configurations on the screen of a DN3500 Apollo workstation. The motivation was to generate a fast display of output from molecular dynamics or Monte Carlo computer simulations. Input to the program consists of a listing of the Cartesian coordinates of the atomic constituents of the molecules. Options in the program include: 1) number of molecules; 2) plot size; 3) atomic radii; 4) superposition of substrate atomic positions; 5) viewing angle; and 6) color-coded and/or numbered atoms. The program is written in Fortran.

Introduction

In computer simulations of molecular systems it is often necessary to display the atomic configurations. Plotting routines, such as those for the Hewlett-Packard (HP) plotters, are slow and take considerable time -- especially when the molecular system contains 100 or more atoms. In water systems one has three atoms per molecule and the number of atoms soon becomes large. The motivation for this work was to develop a plotting routine which would display #600 atomic configurations in a few seconds on the screen of an Apollo DN3500 workstation. In comparison, the HP plot takes about 30 minutes.

Description of the Plotting Routine

The basic plotting routine, called MASTERPLOT, is a Fortran code developed for the HP plotter. It reads the atomic coordinates and plots the atomic configurations in layers, so that the circles representing atoms in the bottom layers are hidden. The present work modified this code to send the output to the Apollo screen. In this version, the hidden line plotting was done by using filled circles for each atom, so that atoms in upper layers covered the circles lying below. The basic program also plots (if applicable) atoms of a substrate in contact with the molecular system.

One of the complications of this project was to make use of the multiple windows available on the Apollo with a mouse based operating system. Each plot appears in a window which can be re-sized with the mouse. The program rescales the output to fit in the new window by selecting a "REDRAW" option with the mouse. By opening new shells, one can display multiple plots and compare rotated or later time views of the atomic configurations. Many of new routines were developed from variations on code provided by the Apollo graphics manual.

An example of the plot, applied to water molecules is shown in Figure 1. Three plots are shown: a) a view looking down (along the -z axis) on 96 water molecules adsorbed on a model AgI substrate; b) the same system looking along the y axis; and c) a plot of the molecular density perpendicular to the substrate. The information in part c) of Figure 1 must be read into the program in a separate file.

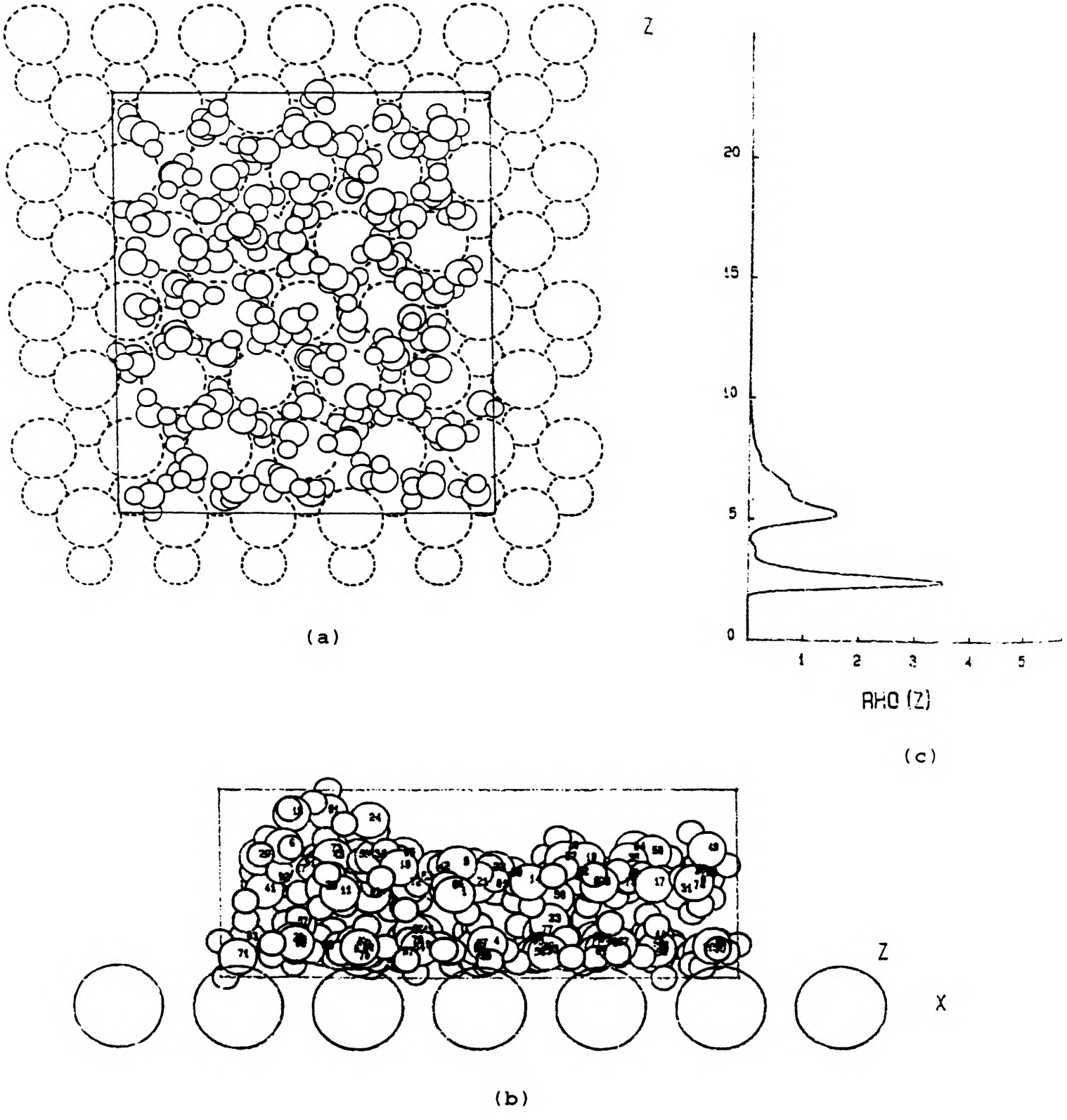

Figure 1

The Fortran Code

The code was written for the Apollo operating system SR 10.1. Modifications for later versions of the operating system should require minimal effort. However, if applied to the new HP-Apollo UNIX workstations some more extensive changes might be required.

Part of the Fortran code is given below, showing definition of input variables, dimensions of the arrays and open and close statements for files. A diskette containing the file can be obtained from B. Hale, Physics Department, University of Missouri-Rolla, Rolla, Missouri 65401.

Summary and Comments

This project, completed during the summer of 1990, was sponsored by the University of Missouri-Rolla undergraduate research program. It provided an opportunity to become familiar with the Apollo workstation, its operating system and some of the subtleties of screen graphics. In addition, the routine will be made publicly available. A diskette containing the file can be obtained from B. Hale, Physics Department, University of Missouri-Rolla, Rolla, Missouri 65401, or by sending a request message to hale@apollo.physics.umr.edu.

This computer graphics program displays water molecule configurations on the screen of a DN3500 Apollo workstation. The motivation was to generate a fast display of output from molecular dynamics or Monte Carlo computer simulations. Input to the program consists of a listing of the Cartesian coordinates of the atomic constituents of the molecules. Options in the program include: 1) number of molecules; 2) plot size; 3) atomic radii; 4) superposition of substrate atomic positions; 5) viewing angle; and 6) color-coded and/or numbered atoms. The program is written in Fortran.

```
C*********************************************************************
C****** PROGRAM: APOLLOPLOT              DATE:Spring/Summer 1990     ****
C******    Prev. MASTER PLOTPORT A       DATE:DECEMBER 1982          ****
C******          (HEREIN REVISED FOR APOLLO COMPUTER)                ****
C******          (Prev. REVISED FOR PC AND IBM 6 PEN PLOTTER)        ****
C******    NOTE: LIMIT = 200 WATER MOLECULES  (7-8-87)               ****
C*********************************************************************
C****** VERSION 1 - WAYNE JOUBERT (CALLED PLOT 3D A) JULY 1981        ****
C****** VERSION 2 - CHANGES 12/82  (SEE C&*****): R. WARD            ****
C****** VERSION 3 - D. REAGO;  D. SIMKINS FOR NCAR; ADDED RHO(Z)     ****
C****** VERSION 4 - FOR PC BY B. HALE  JULY 1987 (SEE C.....)       ****
C.....     "       USING R. WARD'S OAK RIDGE VERSION (DRAWHP.FOR)   ****
C.....     "       DOES NOT DRAW TO MONITOR SCREEN                  ****
C****** VERSION 5 - FOR APOLLO BY M. STULLER BASED ON ROUTINES BY    ****
C.....     "       M. STULLER AND A. GAUS.  DRAWS ON APOLLO SCREEN.****
C*********************************************************************
C****** DESCRIPTION OF INPUT DATA                                     ****
C&***** IPEN = 1 PLOTTER PEN DOWN; =2 PLOTTER PEN UP                 ****
C&***** INK PENS (CANNOT BE USED ON 1051 PLOTTER)                    ****
C****** NMOL = NUMBER OF MOLECULES                                   ****
C****** SIZE = WIDTH OF SQUARE PLOT IN CM;  =FLOAT(INTEGER LE.15)    ****
C****** IDISK = 1 READ FROM SEPARATE FILE 18, =0 READ FROM FILE 7    ****
C****** INFO = 1 PRINT INFO ON PLOT, = 0 DONOT PRINT INFO            ****
C****** INUMB = 1 PUT NUMBERS ON MOLECULES, =0 DON'T NUMBER          ****
C******          ****** no longer in use  - 8/90 *****              ****
C****** IBOX = 0 NO BOX, = 1 BOX DRAWN; BOX = ~UNIT CELL             ****
C****** IBOX = 2 DRAW CIRCLE OF RADIUS RAD AT CENTER MASS (XCEN,YCEN) **
C******           (CALCULATED IN SUBROUTINE  GETHTO)                ****
C****** ISKIP = 1 EXTERNAL SCALING, 0: AUTO. SCALING (IN PROGRAM)    ****
C****** RMN,RMX = MIN AND MAX FOR EXTERNAL SCALING IF ISKIP = 1      ****
C..... IRHO = 1 PLOT RHO(Z); =0 NO RHO(Z) PLOT                      ****
C****** ISUB = 0- NO SUBSTRATE,1- AGI ,2- PRISM ,3- LJ93             ****
C****** XSUB,YSUB,ZSUB = LOCATION (IN ANGSTROMS) FOR TOP OF SUBSTRATE **
C******          (FOR LJ93 XSUB,YSUB HAVE     NO MEANING (ENTER 0.,0.)****
C******           ZUB = 0.0 FOR ALL OF OUR SET UPS                  ****
C****** PSPC = PERSPECTIVE VALUE >0. IS DISTANCE IN ANGSTROMS ABOVE ICE
C******         LATTICE, VALUE <0. NO PERSPECTIVE APPLIED,          ****
C******         CLUSTER IS CENTERED AT (0.,0.,0.) IF PSPC IS >0.!!  ****
C&***** ICENTR = 0 DO NOT CENTER CLUSTER; = 1 CENTER CLUSTER         ****
C&*****          (ONLY USED IF PSPC IS <0.)                         ****
C****** NVIEW = 1,2,3 ==> XY, ZY, ZX VIEW GENERATED IN THIS VER.     ****
C****** XANG,YANG,ZANG = ANGLES OF ROTATION ABOUT FIXED X,Y,Z AXIS   ****
C&***** TEMP,NSTEP = TEMPERATURE AND MONTE CARLO STEP #              ****
C..... BORDER =BORDER (ANGSTROMS) BEYOND UNIT CELL FOR PLOT REGION  ****
C..... EDGE = DISTANCE BEYOND X,Y MIN,MAX TO SPECIFY A UNIT CELL    ****
C..... VS = PEN SPEED, (0 TO 127.999 CM/SEC )                       ****
C..... IPENH,IPENO=H, O PEN COLOR: 1,2,3,4,5,6=BLK7,R,G,BL,BR,BLK3  ****
C..... RHYD,  ROXY  = RADII FOR H AND O, IN ANGSTROMS (0.5,0.74)    ****
C..... ICHP = PEN COLOR FOR LEGEND, SUBSTRATE; SET = 1              ****
C..... NCOM1 = 0 , 1 ==> OUTPUT TO DISKFILES, COM1(TO PLOTTER0      ****
C..... IKEMP = 0 , 1 ==> READ COP,CHAP,CHBP 3(E14.7,2X),3(E15.8,2X)****
C..... ITEST = 0 , 1 ==> WRITE DETAILS OF PLOT OUTPUT, NO WRITE     ****
C*********************************************************************
C
C       Apollo-specific Variable Descriptions:
C
C               main_window_dim     array containing x origin, y origin, width, and
C                                   height of the main window used for graphics
C
C               main_window_id      an IOS stream identifier for the main window
C                                   (acts much like a device number in FORTRAN)
C
C               main_window_pm      a GPR identifier for the bitmap associated with
C                                   the main window (this bitmap can be saved on file)
C
C                                   If more than one graphics window was being used,
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