COMPUTER SYSTEMS RESEARCH
Running Version of Your Program, example report form 2007-2008

1. Your name: Ben Parr Period: 6
2. Date of this version of your program: 1/23/08
3. Project title: Accurate 3D Modeling of User Inputted Modeling Using a Hill Climbing Algorithm
4. Describe specifically what files are needed and the command(s) necessary to run your program

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    How to run your demo:

In order to compile the program, these files are needed:
   1. main.c (conptains my main funtion which starts OpenGL)
   2. initicalize.c (initializes all global variables and OpenGL)
   3. draw.c (contains functions for drawing the model and positioning the
      eye)
   4. fileWork.c (contains functions to import/export model and get data from
      elements.data)
   5. inputControls.c (handles all inputs from the mouse and keyboard)
   6. drawBonds.c (has functions to draw a single, double or triple bond)
   7. menu.c (creates the menu system, which is attached to the middle
      button)
   8. Lgcc (compiles the program)

Once compiled, these files are needed:
   1. main (executable version of my program)
   2. elements.data (contains information, such as atomic radius, for each
      individual element)
   3. Any file you wish to import as a model
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5. Your program is running, now what? List test input(s) for the user to interact with your program. Specifically what should the user expect to happen?

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      Input(s) = Program's expected response(s):

   1. ./main FILENAME in the terminal) = start my program and import the data
      in the file given
   2. clicking left button and moving the mouse = rotate the model
   3. scrolling up or down on the scroll wheel - zooming in and out on the
      model
   4. pressing '1', '2', or '3' on the keyboard = changing the type of bond
      that will be drawn
   5. right click on an atom or bond = select that atom or bond
   6. pressing the 'Back Space' or 'Delete' button = deletes the selected
      atom or bond
   7. clicking the middle/scroll button = activate menu system where you can
      import/export a model or select the element you want to draw
   8. left click while holding the 'Ctrl' key = create a new atom
   9. right click while holding the 'Ctrl' key = create a new bond
   10.left click while holding the 'Shift' key = move the selected atom
      based on movements of the mouse
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6. What about user input errors? Are there incorrect user input(s) that your program handles?

When given a file to import that doesn't exist, my program Segmentation faults because I could not find a way to check to see if the file exists in C. This is the only input error that is not handled. My program does nothing when the given other incorrect user input.

7. What is the programming doing, demonstrating, or analyzing? What is the user looking for in order to understand what you've been studying and developing with this project?

My program allows users to easily create and view simple molecules (i.e. not macromolecules). Therefore, the user is looking for an easy and intuitive user interface to allow for the easy creation of molecules. Programming this interface has been my main focus of the second quarter.

8. How has your program evolved during second quarter to now, the beginning of third quarter?

I have programmed basically all of the graphics and user interface for my program. At the start of the second quarter, the user could only create atoms and bonds by changing the source code. The user could also only create single bonds. The program also had the ability to rotate and zoom. Now users can create molecules while running the program. While running the program, the user can create atoms and bonds, select and delete atoms and bonds, import and export models, draw single, double and triple bonds, choose which element they want to draw, and position the atoms where they want. All of these features were programmed during second quarter.

9. By the end of this school year, what do you hope to have as a final version of your program in relation to this current version? What will you demonstrate during your final presentation?

By the end of this school year, I hope to have a program with an easy and intuitive user interface that would allow a user (mainly a beginning chemistry student) to create a model. Then, with the click of a mouse, have the program position the atoms correctly. During my final presentation, I will demonstrate this process of creating a molecule and then having the program position the atoms accurately.