

TJHSST Senior Research Project

3D Modeling of Molecules

2007-2008

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Abstract

Problem statement and summary of your project's intentions. A brief introduction and overview to the purpose and scope of your research project

Keywords: keywords you'd like to list, ...

1 Introduction - Purpose and Scope

Purpose.

* What is the subject of the project; what are the goals; what is the project about?

* Why is the project worth doing; why is it a good topic for the Computer Systems Lab?

* Who will be interested in the results; how can the results be applied?

Scope of Study. Describe the overall bounds of the work that will be involved, e.g., the research or data that will be required, and the relationships and variables that will need to be programmed, and the expected results

* For example: Students may experience difficulties finishing their projects because of the complexities they encounter. In this case, you may have to narrow down your research/project objectives.

* Be as specific as you can about what you want to develop. Think of drawing a boundary around the area of study that you think you can finish.

* If your project idea is too extensive, select a more modest piece of your original project idea to work on.

2 Background

Background and review of current literature/research in this area.

* Demonstrate that you have looked into and read about the background area of your topic.

* What kinds of research have been done before in this area? How have others gone about trying to solve similar problems you are interested in?

* Is there a "state of the art" today? (Ex. "I want to write a search engine"...Google would represent a state of the art version)

* In what ways may your approach build on and vary from previous work that has been done in your project area?

* Think about a bibliography: references in this background and literature review section can be in your bibliography, but not everything that will be in your bibliography needs to be included here.

3 Procedures

Procedure and Methodology

* Show that you clearly understand your task and have a logical time plan for your research and reading, design for implementation, programming of your implementation, and testing phases of your project.

* Show that you have identified the resources you will need.

* What tasks will have to be accomplished to meet your objectives?

* What materials and programming language(s)/tools will be necessary?

* What visuals can you construct - charts and graphs that aid in portrayal of the information your program is generating

* What input data may be needed, and how will you collect this data?

* What methods and processes will be used to test and analyze your program's performance? What types of error analyses can you do?

3.1 Testing

1. Dynamic testing: random types of input to your program, specific structural and functional testing (how you verify particular sections of your program are working correctly), path and branch testing (picking particular inputs that test internal paths of performance of your program)
2. Process modeling: determining mathematical formulas that can be used to validate the performance of your program, check the predictive quality of your program. For example, how well does your program model existing or expected phenomena, and how well your program may be used to predict behaviors based on future input
3. Requirements and specifications: Defining requirements for your program and the structure of your program, outlining these requirements in written form, and defining specifications you can use for verifying how well your actual program meets these requirements.

* How will you write up your time lines for project development (for example - Gantt charts)?

I plan on using the following tools and sticking with the proposed time scale below.

3.2 Software

Computer language(s) I'll use

- 1.
- 2.
- 3.

3.3 Algorithms/Programs

I'll be using the following algorithms/programs, in addition to designing my own:

- 1.
- 2.

4 Schedule

In the first quarter, I will focus on ...

In the second quarter, I will begin to research one or more data types that I hope to use for ... I will have to learn how to ... A program at this point would ...

In the third quarter, I will bring together both earlier parts to form a complete ... application. It will be able to ...

5 Expected Results

Expected Results and Value to Others

* What results do you expect to obtain from your project?

How will the final results and analyses be presented (include visuals such as graphs and charts)?

Can you think of particular contributions these results can give to future researchers?