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**Senior Capstone Systems Requirement Document**

**User Requirements**

We will be developing a molecular dynamics simulator that will be implemented using the Metropolis Monte Carlo method. This system will show students how statistics relates to chemistry, and will be able to give students a computer generated design of molecular motion on an atomic scale. This system will consist of 5 basic sets:

* Step 0: Pick initial configuration
* Step 1: Random number conforms to particle
* Step 2: Generate random number to tell you how far to move particle
* Step 3: Calculate the new energy of the system, ∆E-Enew - Eold
* Step 4: if ∆E < 0 Accept the move and go back to step 1

if ∆E ≥ 0 (acceptance probability p= e^(-β∆E) β = 1/kT

K = Boltzman's constant

T = temperature

Boltzman’s Constant= 1.3806503 × 10-23 m2 kg s-2 K-1

Generate r is R ≤℮^(-β∆E) accept the move + go to step 1

R >℮(-β∆E) reject move go one step back

Keep track of the number of accepted and rejected moves

**System Requirements**

* Will run on a Linux based OS
* Will be coded using C++ and will have ability to be displayed in 3 dimensions
* Will be implemented using Metropolis Monte Carlo

**Functional Requirements**

* Prints out configuration every x amount of steps
* Will allow an input file and User will be able to edit the input file before running.
* Outputs data to a .xyz file for simulation on VMD.
* Will be able to run off a student crafted text file, or from a txt file created by the GUI.
* Will have a Graphical GUI interface which creates a text file for input to the algorithm, it will also display the graph of the energy.
* Will have a restart option allowing the user to start over and also start where they left off
* Header will be printed in the output file which will give user information about what the input file contains

**Non-Functional Requirements**

*Organizational Requirements*

* Use of C++
* Use of Linux

**Domain Requirements**

* The output of the program will have three files, an .xyz file for movie playback, which uses VMD, a .csv file for the graph for the energy levels and a .txt file containing configuration information.

**System Model**

**Energy**

*Energy Difference  
Compare if E<0  
If YES*

*Create Box  
Create Particles*

*Create Random No.  
Pick Particle  
Move Particle*

**Initial Configuration** **Random No.**

*User Input  
Input File*

*After cycle completion*

**Save Con.**

**Output** **Load Last Config**

If NO

*Compare probability  
Create Random No.  
Compare R<=P  
If YES*

If NO

*After certain no. of cycles*

**Probability**

**Snapshot**