Workplan Project ‘Molecular Mechanics’

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In this project, code will be written for the parametrization of an energy function from a given molecular structure, consisting of only hydrogen and carbon atoms, and is minimized. Here, a workplan is proposed.

The code will consist of three modules and one main program. The three modules will be split in the following branches (see next page for visualization):

- **The module ‘Atom’**. Here, a type ‘Atom’ is created which can store the type of atom (H or C) and his Cartesian coordinates. It also contains a subroutine ‘ReadData’, which reads the input from a file and stores the values into type ‘Atom’. Another thing the subroutine initiates is the storage of all the used parameters in the model.
- **The module ‘Energy’**. This module contains all the subroutines being used to calculate the different types of contribution to the energy, as well as the subroutine which combines all these subroutines to calculate the total energy of the system.
- **The module ‘Minimization’**. This module contains only one subroutine called ‘Move’. In this subroutine, the already known total energy of the current configuration is stored first in a dummy variable. Then, a random atom of the system is moved according to a random vector and the total energy of the new configuration is calculated and stored. In the final steps, with the value of the new and old energy, it is checked if the new configuration is accepted with a probability function. If it is accepted, the new configuration is saved and the ‘Move’ subroutine is called again until you reach an amount of cycles, which I will call the exit strategy for now. This exit strategy is coded in the main program.

On the next page, the three modules are visualized and there is a flow chart given of the main program. The first step of the main program will be the initialization of the system by reading in all the data about the atoms and parameters by calling the subroutine ‘ReadData’. In the next step, the total energy is calculated of the initial configuration and stored in a temporary variable called ‘StartEnergy’. Then, the subroutine ‘Move’ is called in order to minimize the energy function. To break the loop, the exit strategy is used. One method that seems suitable to me is to keep track of the amount of times the configuration of the molecule isn’t changed. After a certain amount of consecutive unsuccessful moves, there could be concluded that the energy function is a minimum. When this is finished, the value of the minimized energy is printed out.

Module Atom

- Type Atom
  - Type of atom (H or C)
  - Coordinates (x,y,x)
- Subroutine ReadData
  - Stores it in Atom
  - And stores all the parameters

Module Energy

- Subroutine StretchEnergy
- Subroutine BendingEnergy
- Subroutine TorsionalEnergy
- Subroutine NonBonded
- Subroutine TotalEnergy
  - Combines the other subroutines

Module Minimization

- Subroutine Move
  - Call TotalEnergy (give name OldEner)
  - Select random particle
  - Give particle displacement
  - Call TotalEnergy (give name NewEner)
  - Check if new position is accepted with probability formula
  - If accepted, save the new configuration for the next displacement