Documentation Molecular Mechanics Project

* 1. **Modules**
  2. **Constants**

This module defines physical and molecular constants for molecular simulation calculations.

* 1. **EnergyCalculations**

This module contains procedures to calculate energy components from a molecule's structure.

* 1. **HelperCalculations**

This module contains helper functions for geometric and bonding calculations.

* 1. **IdentifyInteractions**

This module contains procedures to identify existent bond patterns in a molecule.

* 1. **InputOutput**

This module contains subroutines for reading molecular data from files and writing output.

* 1. **MetropolisAlgorithm**

This module contains a subroutine to minimize an energy value using a Metropolis algorithm.

* 1. **MinimizationExperiment**

This module coordinates a comprehensive molecular minimization experiment by optimizing energy configurations.

* 1. **Types**

This module defines the types for atoms, bonds, angles, dihedrals, and nonbonded interactions.

* 1. **VectorMath**

This module contains procedures to perform calculations between two vectors.

1. **User-Derived Data Types**

The user-derived data types can be found in the Types module.

* 1. **Atom:** Defines the Atom type for representing individual atoms and their properties. Contains properties unique for a specific atom type (C or H).
  + **type** (character: ‘C’ or ‘H’)
  + **x, y, z** (real(kind=8): Cartesian coordinates)
  + **R\_nb** (real(kind=8): Lennard-Jones parameter)
  + **epsilon\_nb** (real(kind=8): Lennard-Jones parameter)
  + **q\_nb** (real(kind=8): partial charge)
  1. **Bond:** Defines the Bond type for representing covalent bonds between atoms. Contains properties unique for a specific bond type (CC or CH).
  + …
  1. **Angle:** Defines the Angle type for representing angles formed by three atoms. Contains properties unique for a specific angle type (CCC, CCH or HCH).
  + …
  1. **Dihedral:** Defines the Dihedral type for representing torsional angles formed by four atoms. Contains properties unique for a specific dihedral angle type (CCCC, CCCH or HCCH).
  + …
  1. **NonBonded:** Defines the NonBonded type for representing nonbonded interactions between atoms. HCCH). Contains properties unique for a specific nonbonded pair (CC, CH or HH).
  + …

1. **Procedures**

- Subroutines and functions

1. **Interdependencies**

**4.1. Data Flow Diagram**

The interdependencies between the different modules are presented in **Figure 1**. **Afbeelding met tekst, schermopname, Lettertype, diagram

Automatisch gegenereerde beschrijving**

Figure 1. Data flow diagram of the modules in this Molecular Mechanics project.

The *MinimizationExperiment* module contains the subroutine *RunMinimizationExperiment(inputFilename, outputFilename, T, r, tolerance, maxIter)*, which is called in the main program.

1. **Input and Output**

- Input/Output handling