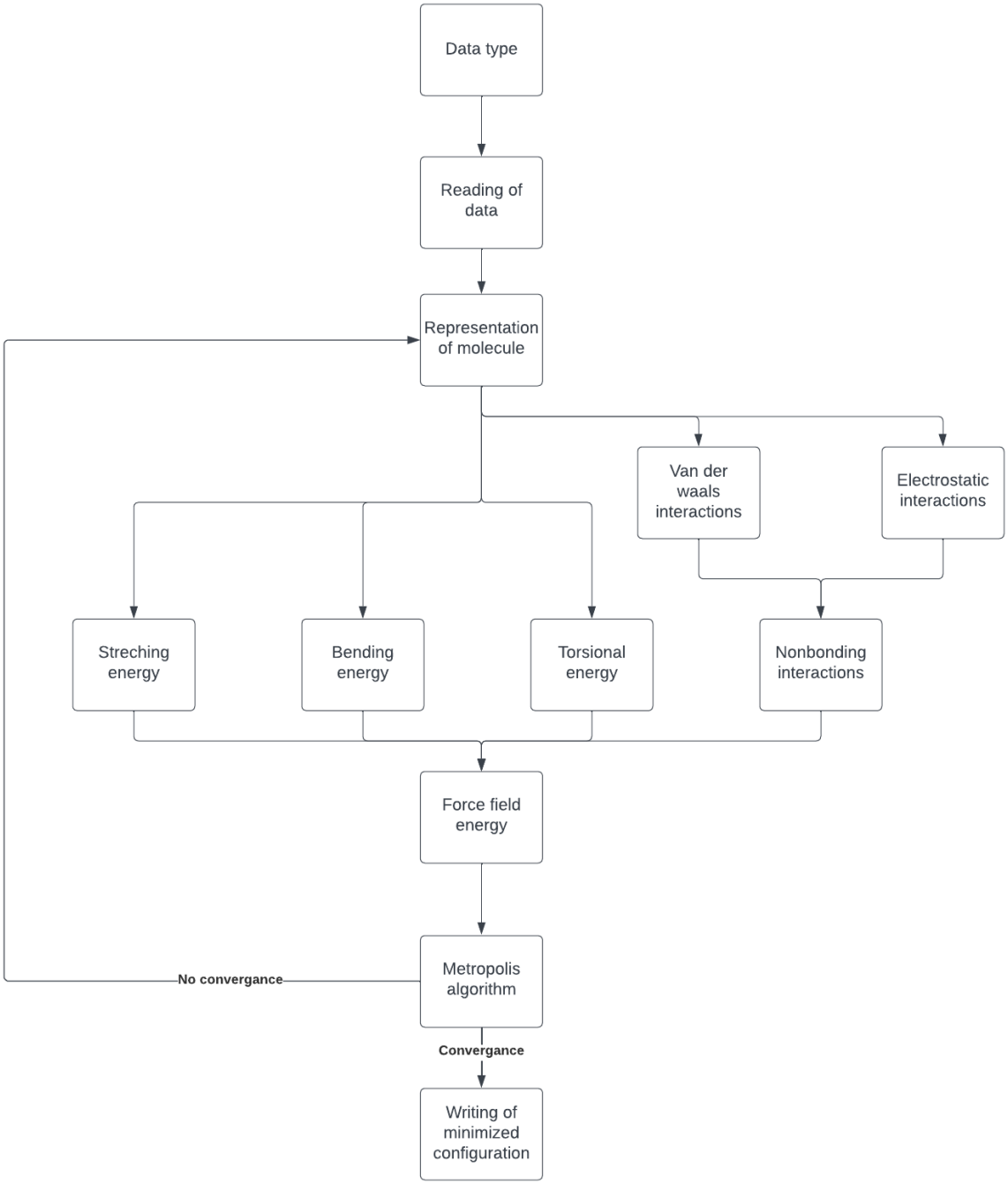
Data type
Reading of data
Representation of molecule
Van der waals interactions
Electrostatic interactions
Streching energy
Bending energy
Torsional energy
Nonbonding interactions
Force field energy
Metropolis algorithm
No convergance
Convergance
Writing of minimized configuration

Data types:

```
type atom
! Setting the element in this project only C (carbon) or H (hydrogen)
character(1) :: element = 'E'
! The xyz coordinates of the atom in the molecule
real(realkind) :: cords(3) = 0.
end type

type bond
! Setting the indices of the atoms that are bonding
integer :: link(2) = 0
! Setting the type of bond in this project only CC or CH
character(2) :: type = 'EE'
! Setting the calculated distance of the bond in A
real(realkind) :: length = 0.
! Setting the vector for the bond
real(realkind) :: vector(3) = 0
end type

type bond_angle
! Setting the types of bonds over which the angle is calulated
character(2) :: bonds(2) = (/'EE', 'EE'/)
! Setting the indicies of the atoms over wich the angle is calcualted
integer :: atom_indicies(3)
! The actual angle of the bonds
real(realkind) :: angle = 0.
end type

type molecule
type (atom), allocatable :: atoms(:)
type (bond), allocatable :: bonds(:)
type (bond_angle), allocatable :: angles(:)
end type
```

is it better to make a type called molecule under which the different data types are placed (atom, bond?

What does R0AC2 mean

What does lower case omega mean (angular frequency)

Non bonding interactions

How to minimize? By changing coordinates

Metropolitan with random distribution?