Flowchart Molecular Mechanics

```
┌─────────────────┐
│   Read Input    │
└─────────────────┘
         │
         ▼
┌─────────────────┐
│   Store data    │
└─────────────────┘
         │
         ▼
┌─────────────────┐
│ Calculate Total │
│     Energy      │
└─────────────────┘
         │
         ▼
┌─────────────────┐
│ Choose a new    │◄──────────────┐
│ vector          │               │
└─────────────────┘               │
         │                        │
         ▼                        │
┌─────────────────┐               │
│ Calculate Total │               │
│     Energy      │               │
└─────────────────┘               │
         │                        │
         ▼              YES   ┌──────────────────┐
┌─────────────────┐────────► │ Replace old      │
│ Accept New      │          │ position by new  │
│ Position?       │          │ position         │
└─────────────────┘          └──────────────────┘
         │ NO
         ▼
┌─────────────────┐
│ 'NO' 100 times  │
│ in a row        │
└─────────────────┘
         │
         ▼
┌─────────────────┐
│     Print       │
└─────────────────┘
```
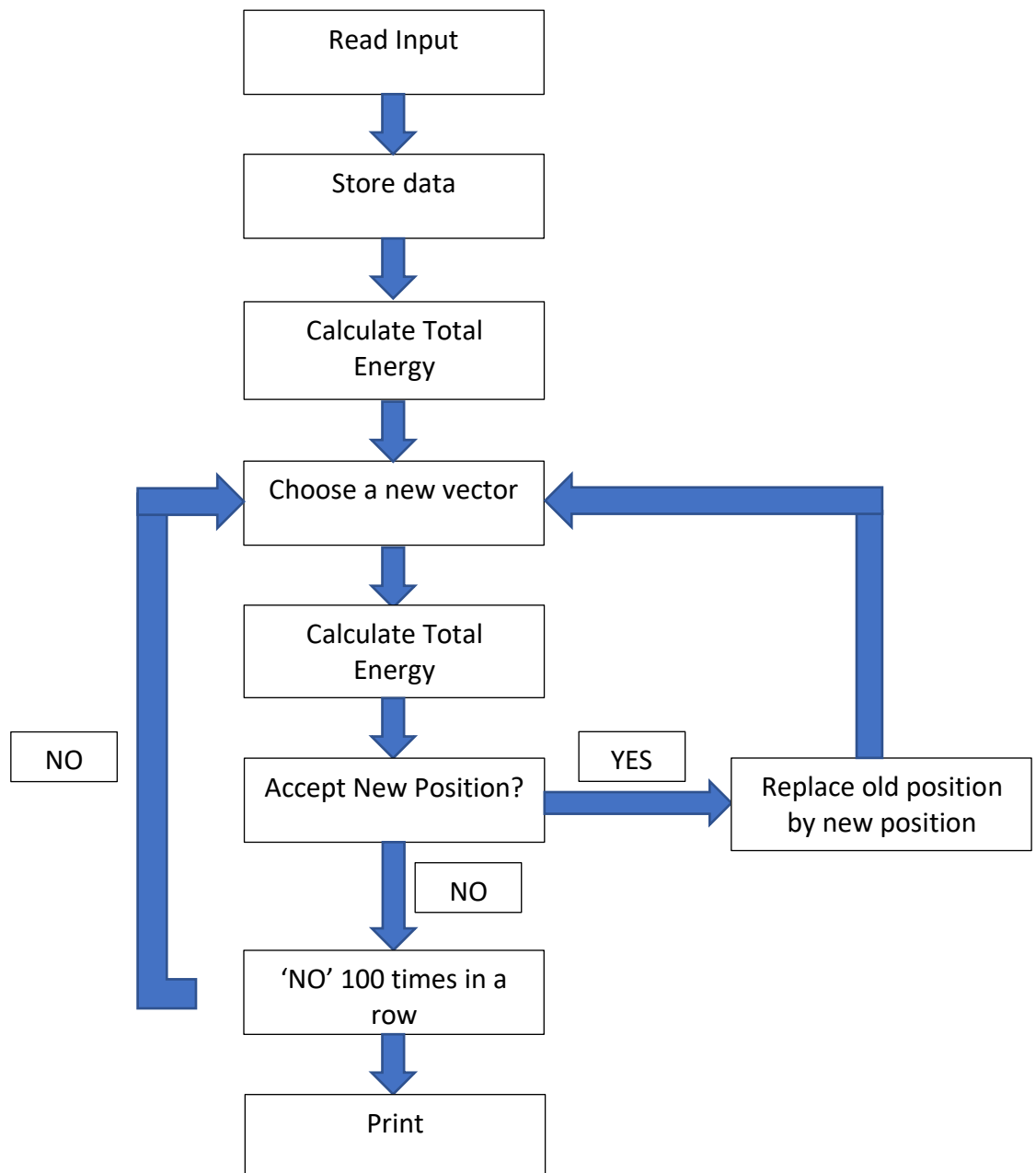
NO

Project backbone

This project will contain three modules and one main program.

Module "AtomReader"
This module reads the input file and stores the data parameters of the atom using types.

Module "EnergyCalculation"
This module calculates the energy by using the 5 given formulas each in different functions.
The "energycalculation" takes as input the data parameters and outputs the total energy.

Module "EnergyMinimization"
This module moves the configuration by choosing a new vector of data parameters,
calculates the total energy and the energy difference. If the new configuration is accepted,
then this will replace the old configuration. Otherwise, the old configuration will be kept. If
the configuration does not change for 100 times the loop will be stopped.