Implementation of Go language to calculate ground state energy of atoms based on Density Functional Theory (DFT)

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Abstract. This study is using Go programming language that support parallel programming for numerical calculation. The program was created is designed for calculate ground-state energy of electron, which is based on Density Functional Theory (DFT). The basic mathematics of this program is using many basic concept of numerical mathematics (matrix calculation, Poisson solver, and standard routine of numerical mathematics).

1. Research Background

Processor is the part of the computer that acts as the brain. The function of processor is to handle the speed of processing data, executing user commands, and the ability of the computer to run multiple tasks together (multi-task). Speed and multi-task are depends on a part of the processor called core. The processor expanding the development by add number of cores that construct it.

The development of the processor and the number of cores can increase the performance of calculation and reduce calculation time. It is because the elements of the processor can do different tasks at the same time (multi-tasking). The multi-tasking process is supported by many core systems. Multi core systems are the right solution when users want to increase high processing speeds, for example in numerical calculations.

In addition to cores, supporting programming languages also affect the speed of numerical calculations [7]. There are programming languages that are often used for numerical calculations, such as the Fortran, Python, Pascal, and C programming languages. Besides the programming language, there is a new programming language called Go. The process of Go language compilation is faster than C language [6]. In addition, the Go language also supports multiple core systems, making it suitable for numerical calculations. **Error! Reference source not found.**

This study utilizes the Go language as a programming language in DFT-based calculation programs. The aims of the program is to calculate the ground state energy of simple atoms

2. Calculation method

The program is designed by implementing DFT to the Go programming language. The program divided into four processes that we specify, such as Figure 1. Process A determines the initial electron density (ρ_N). Process B determines the potential energy of the electron (V). Process C determines the ground state energy (E_N). The D process determines the new electron density (ρ_{N+1}) for the iteration process. If the fourth process has finished, the program will iterate. The output in the fourth process will be input to the second process, replacing ρ_N in the first process.

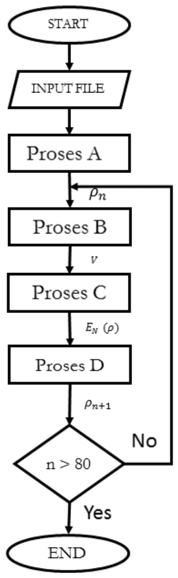

Figure 1. Flow chart of the program based on DFT calculation

The flow chart that have designed is then used to build a ground state energy calculation program using the Go programming language. The program is tested on a number of selected atoms, such as: H, He, C, O, Cl, Fe, and Zn. The results of testing the calculation atoms compared with the results obtained using the C language program.

In addition to getting the energy, we also get the program calculation time. So we also compare the time needed by the Go language and the C language for the calculation of each atom.

3. Result and discussion

3.1. Flow diagram based on DFT

The flow of this program started with process A is to determine the initial electron density (ρ_N) of an atom tested. In Figure 2 shows the program flow to determine ρ_N. It is seen that to determine ρ_N requires an atomic number (Z), the maximum number of orbitals (nmax), the maximum number of angular momentum (lmax), and the number of electrons that fill each atomic skin (F [l] [n]) as input. We get this information from the atomic electron configuration tested.

Furthermore, these inputs are used in four stages. The first step to determine ρ_N is to determine the total energy for all orbitals (E). The Z and nmax values are used as inputs to calculate the energy of each orbital (En). Each En value is n = 0 until nmax is added up, then multiplied by the number of electrons filling the skin (F [l] [n]). So that we get total energy for all orbitals (E).

The second step is to calculate the total effective potential energy of the electron at all angular momentum, which we represent with V_0. Before getting the value V_0, we first calculate the effective potential energy value V_{eff} at each angular momentum. V_{eff} is calculated for each value of l, starting from l = 0 to lmax. The value of V_{eff} for each l is summed then multiplied by the number of electrons filling the skin (F [l] [n]), to get the total potential effective energy (V_0).

Then the third step is to solve the Schrödinger equation computationally. The values E and V_0 obtained from the first and second processes we use to get the wave function ($\psi_0(x)$). From the value of ψ_0 obtained in the fourth stage, we use it to determine ρ_N. The square of ψ_0 gives the electron distribution, the total electron density is the sum of the squares ψ_0 multiplied by the number of electrons that fill the F[[l] [n] orbitals. In mathematical form, electron density is written as follows

$$\rho\,(x) = \sum_i F_i[l][n]\,|\psi_i\,(x)|^2.$$

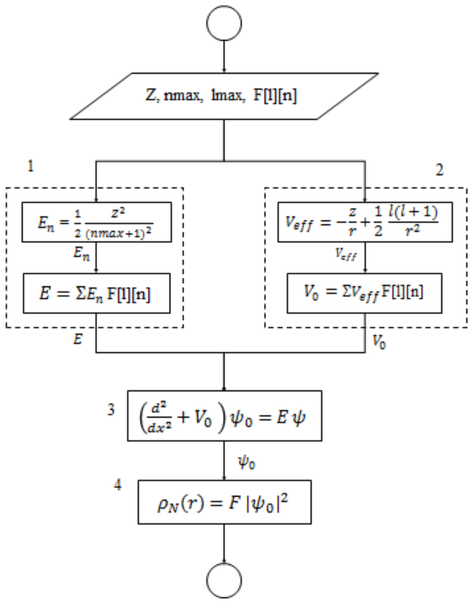
Z, nmax, lmax, F[l][n]
1
2
$E_n = \frac{1}{2}\frac{z^2}{(nmax+1)^2}$
E_n
$E = \Sigma E_n$ F[l][n]
$V_{eff} = -\frac{z}{r} + \frac{1}{2}\frac{l(l+1)}{r^2}$
V_{eff}
$V_0 = \Sigma V_{eff}$F[l][n]
E
V_0
3
$\left(\frac{d^2}{dx^2} + V_0\right)\psi_0 = E\,\psi$
ψ_0
4
$\rho_N(r) = F\,|\psi_0|^2$

Figure 2. Finding initial density

The process of B in this program flow is to determine the potential energy of the electron, such as Figure 3. There are three potential energy contributing here, Hartree potential energy (V_H), potential electron energy with nucleus ($V(r)$), and *exchange-correlation* potential energy (V_{XC}). So that the total potential energy is the sum of the three potential energies.

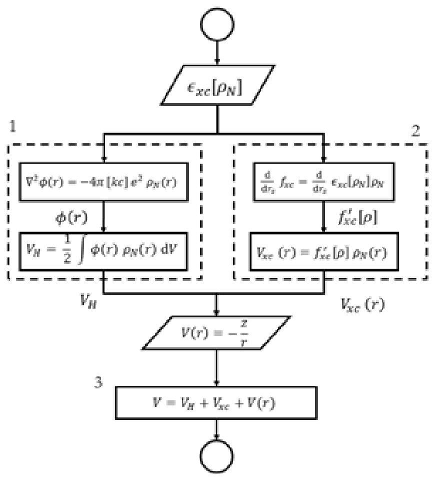
$\epsilon_{xc}[\rho_N]$
1
2
$\nabla^2\phi(r) = -4\pi\,[kc]\,e^2\,\rho_N(r)$
$\phi(r)$
$V_H = \frac{1}{2}\int \phi(r)\,\rho_N(r)\,dV$
$\frac{d}{dr_s} f_{xc} = \frac{d}{dr_s}\,\epsilon_{xc}[\rho_N]\rho_N$
$f'_{xc}[\rho]$
$V_{xc}\,(r) = f'_{xc}[\rho]\,\rho_N(r)$
V_H
$V_{xc}\,(r)$
$V(r) = -\frac{z}{r}$
3
$V = V_H + V_{xc} + V(r)$

Figure 3. B process for finding potential energy

V_H is potential energy from the interaction between electrons and electrons. This potential energy is obtained by solving the Poisson equation, with the form of the Poisson equation

$$\nabla^2 \phi\,(\vec{x}) = -4\,\pi\,[kc]e\,\rho(\vec{x})$$

$\phi\,(\vec{x})$ is electronic potential energy for one electron. So to find potential energy due to the interaction of electrons with other electrons, it needs to be multiplied by the electron density. The mathematical forms of V_H are as follows,

$$V_H = \frac{1}{2}\int \phi(\vec{x})\rho(\vec{x})\,dV$$

V_{XC} is the energy obtained from interactions aside from V_H and $V(r)$. The mathematical form of energy exchange-correlation $V_{XC} = f'_{XC}\left(\rho(\vec{x})\right)$ and $f_{XC} = \epsilon_{XC}\,\rho$. is the mathematical form of the chosen exchange-correlation. We chose the VWN exchange correlation, with a mathematical form

$$\epsilon = A\left[\ln\frac{x^2}{X(x)} + \frac{2b}{Q}\tan^{-1}\left(\frac{Q}{2x+b}\right) - \frac{bx_0}{X(x_0)}\left(\ln\frac{(x-x_0)^2}{X(x)} + \frac{2(b+2x_0)}{Q}\tan^{-1}\left(\frac{Q}{2x+b}\right)\right)\right]$$

if V_{XC} is added to other potential energy it will get total potential energy value,

$$V = V(r) + V_H + V_{XC}$$

The C process in this program is to determine the E_N basic state energy, such as Figure 4 left. If you want to know the energy value, you can use the Schrödinger equation by knowing the value of the wave function and potential energy. Because we already know these two values, we can get the value of E_N, using the Schrödinger equation

$$\left(\frac{d^2}{dx^2} + V\right)\psi_0 = E_N\,\psi_0$$

The fourth process in Figure 4 right of the program flow is to determine the new electron density for the iteration process. The iteration process is carried out to correct the values previously obtained. Because this program is based on an approach, we do iterations as a step to get closer results.

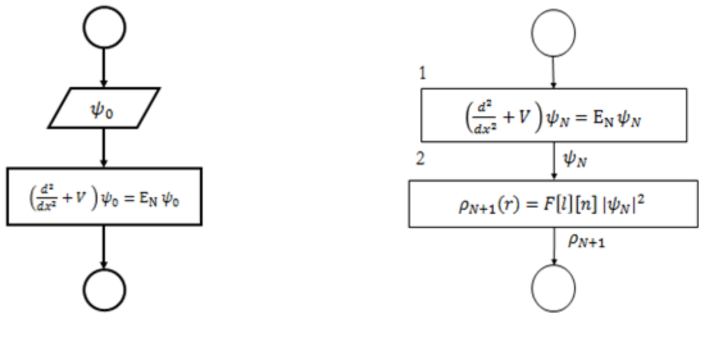
ψ_0
$\left(\frac{d^2}{dx^2}+V\right)\psi_0 = E_N\,\psi_0$
1
$\left(\frac{d^2}{dx^2}+V\right)\psi_N = E_N\,\psi_N$
2
ψ_N
$\rho_{N+1}(r) = F[l][n]\,|\psi_N|^2$
ρ_{N+1}

Figure 4. Left: C Process, Finding ground-state energy. Right: D Process, routine to finding new density

3.2. Program Testing

Based on the program flow that we have designed, we have realized the flow into a DFT-based numerical calculation program. The program that we designed uses the Go programming language. The reason we chose the Go programming language was because according to Peiyi Tang's paper from the Department of Computer Science, the University of Arkansas stated that parallel programming using Go language was easier and more efficient.

We present the program calculation results with the Go language in Table 1. The parameters of the program calculation results that we have tabulated in the table consist of energy values, program calculation time, program number to achieve convergent values, and time taken for the program once iteration. The value we get from the Go language is then displayed in graphical form to see the relationship between the energy value of the program's ability to iterate.

Table 1. The program calculation value

Atom	Atomic Number	Groundstate energy calculation			
		Value (Hartree)	Calcualtion time (s)	N Convergence	Iteration time
Hydrogen (H)	1	-0.44567056136	11.76	25	0.10 - 0.23
Helium (He)	2	-2.83483568022	12.12	29	0.10 – 0.23
Carbon (C)	6	-37.4257485949	32.83	32	0.10 – 1.00
Oxygen (())	8	-74.4730768471	34.97	34	0.10 – 1.01
Chlorine (Cl)	17	-458.664179537	53.55	36	0.09 – 1.01
Iron (Fe)	26	-1261.09305585	15.58	36	0.09 – 1.01
Zink (Zn)	30	-1776.57384967	16.66	37	0.09 – 1.01

Figure 5 shows the graphical relationship between atomic number and iteration convergence. The atomic number axis and Y axis indicate the number of iterations needed by the program to reach convergence. It is seen that the larger the atomic number, the program will need more iterations to achieve convergent values. So the calculated time needed to calculate a large atomic number takes longer.

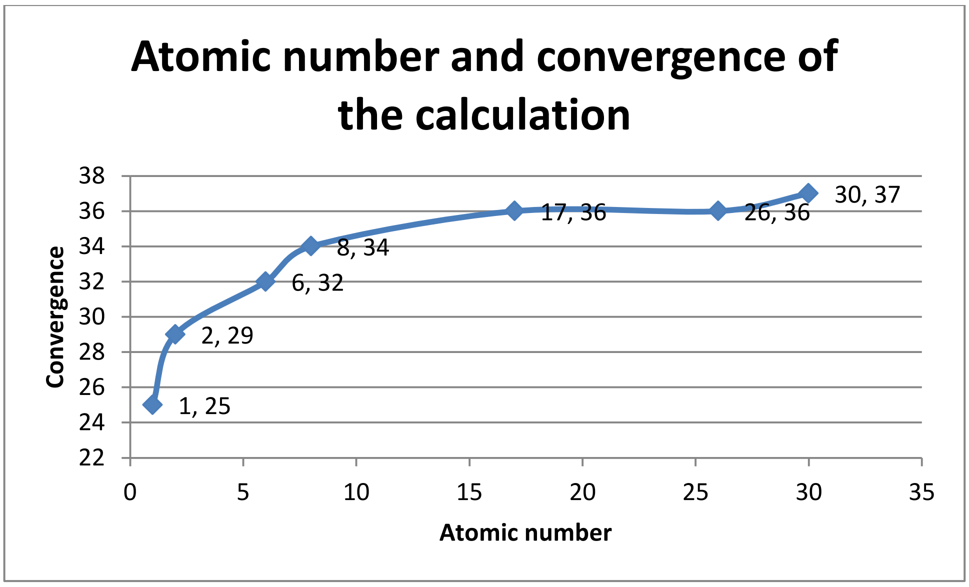

Figure 5. Relation between atomic number and confergence of the calculation

4. Conclution

The Go language program made gives H-atom energy results of -0.45 Hartree with a time of 11.76 seconds; He atom of -2.83 Hartree with a time of 12.12; C atom of -37.43 Hartree with a time of 32.83 seconds; O atom of -74.47 Hartree with 34.97 seconds; Cl at -458.66 Hartree with a time of 53.55 seconds; Fe at -1261.09 Hartree with a time of 15.58 seconds; Zn at -1776.57 Hartree with 16.66 seconds for Zn atoms.

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