Development of Molecular Dynamics Simulation Graphic User Interface by using JAVA GUI Library

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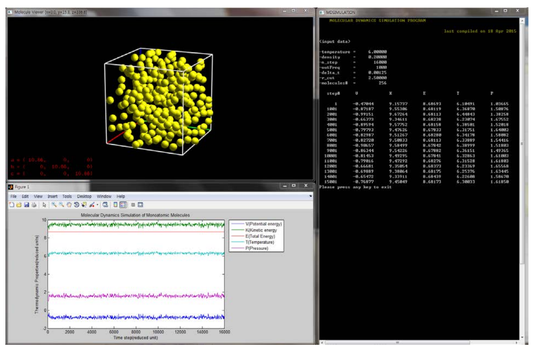
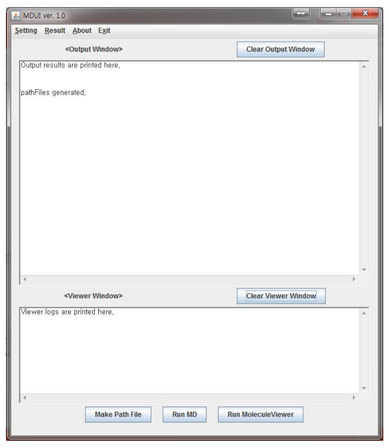
Introduction

▶ Motivation of GUI Development





- Poor accessibility to general users(simulation beginners)
- Hard to organize and manage result data
- Need additional visualization program to monitor the behavior of molecules

Theory

▶ Calculation of Thermodynamic Properties

Initialization : $\vec{r_i}$, $\vec{v_i}$

↓

Force Calculation: $\vec{a_i}$

↓

Integration
(Velocity Verlet Method)

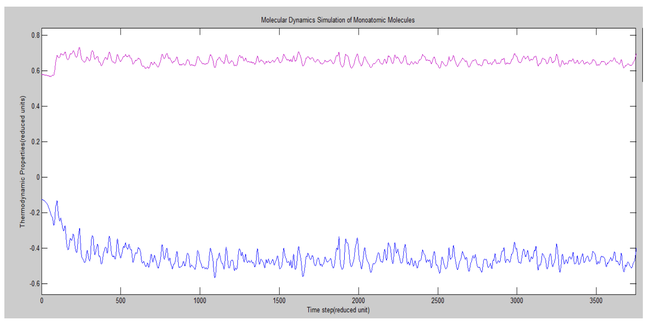
↓

Periodic Boundary condition(PBC)

Program Algorithm

- Minimum Image Convention
- Potential truncation
- Potential, Virial term, Force calculation

Validation of MD Simulation Calculator



temperature = 6.0
density = 0.1
r_cut = 4.0

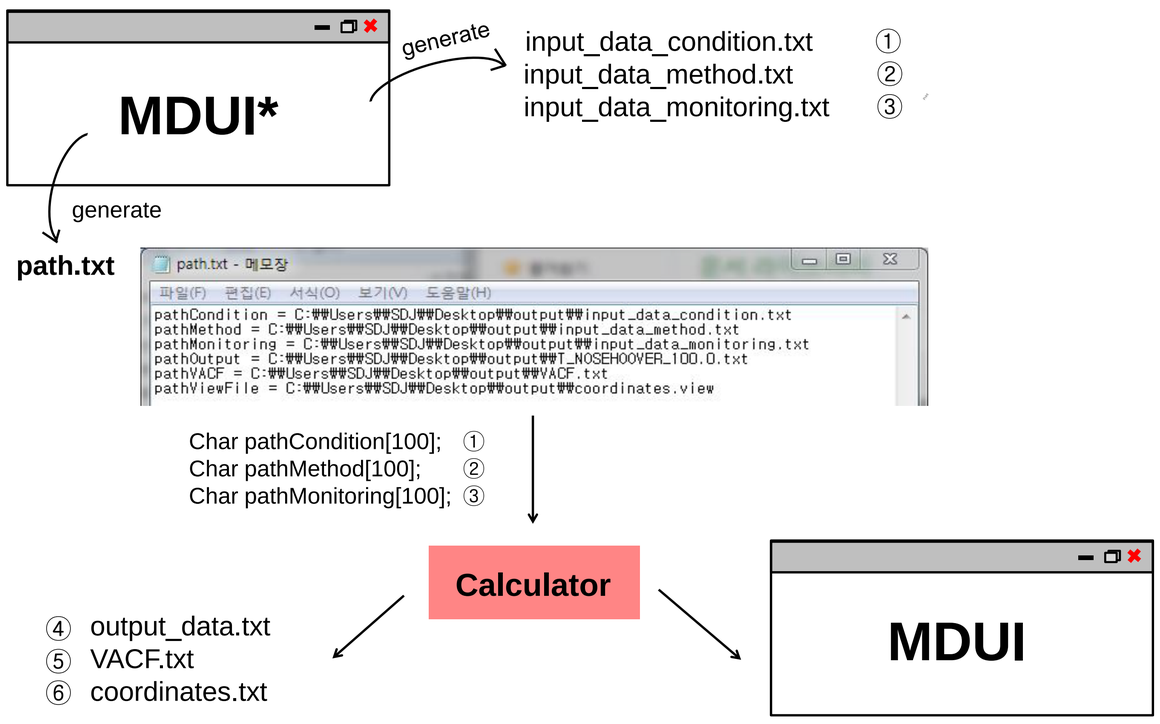
	P*	V*
J. K. Johnson et al.**	0.6499(6)	-0.478(2)
This research	0.6492(5)	-0.475(3)
Error(%)	0.11	0.63

** Molecular Physics, 1993, vol. 78, no.3, 591-618

• The resultant values from the simulation using the MD calculator in NVE ensemble system are in agreement with the reference value in a reasonably small error range.
• Therefore, it was concluded that the C language-based program plays a valid role as a molecular dynamics calculator.

Overall Flow of Data

*Molecular Dynamics with graphic User Interface

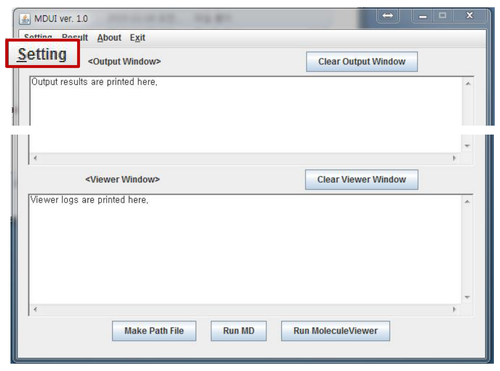


Conclusions

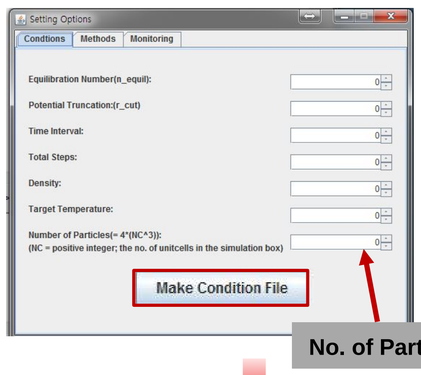
- Runnable on Both Windows and Linux ⟶ Wide accessibility to users
- Automatic generation of folders named as present time and date ⟶ Easy management of data
- Capability to make another simulation program with GUI has been raised during the development procedures
- Additionally, developing scheduling or plotting functions and the capability to deal with various materials are needed

Result (Operation Procedures of MDUI)

▶ Setting Simulation options

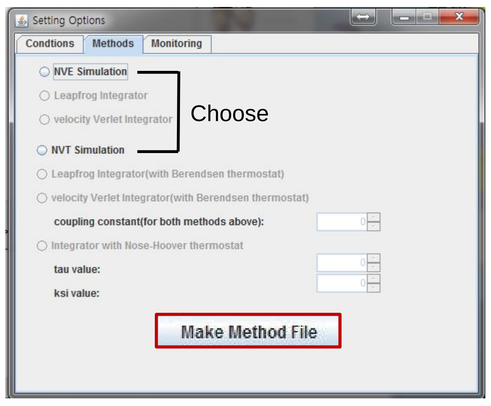


Insert condition value

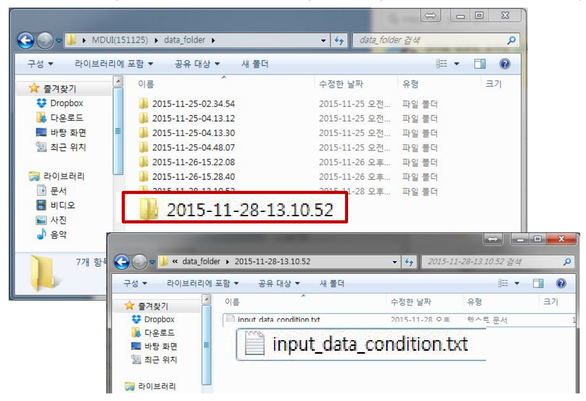


No. of Particle = $4 \times NC^3$

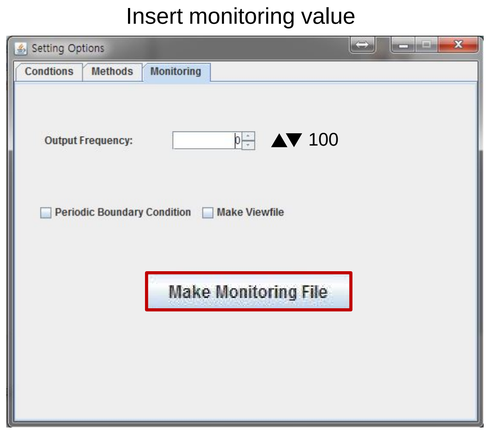
Choose method value



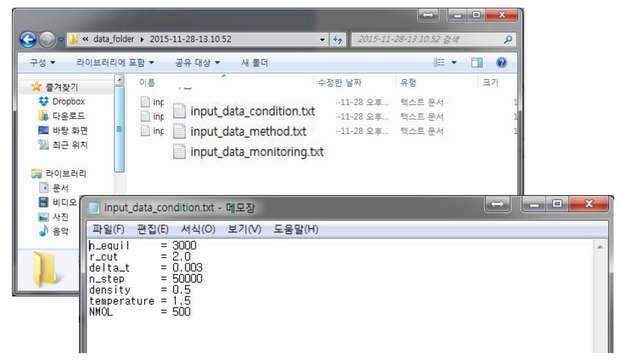
Condition files generated in corresponding folder automatically



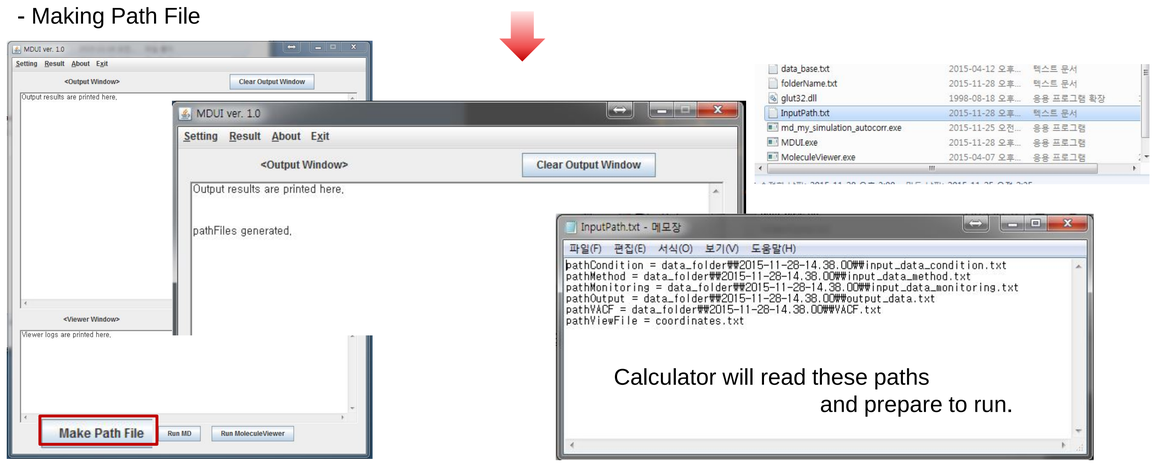
Insert monitoring value



Method and monitoring files generated in corresponding folder

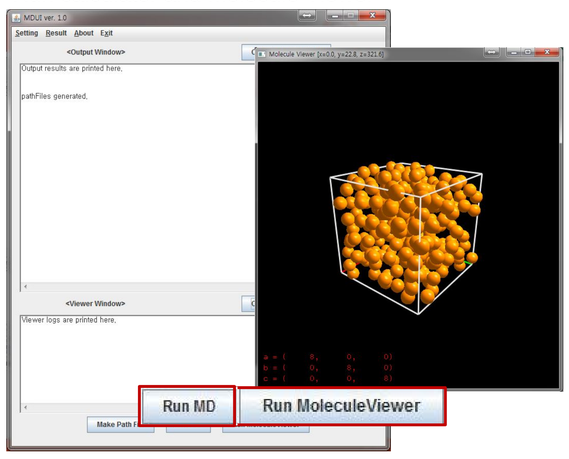


- Making Path File



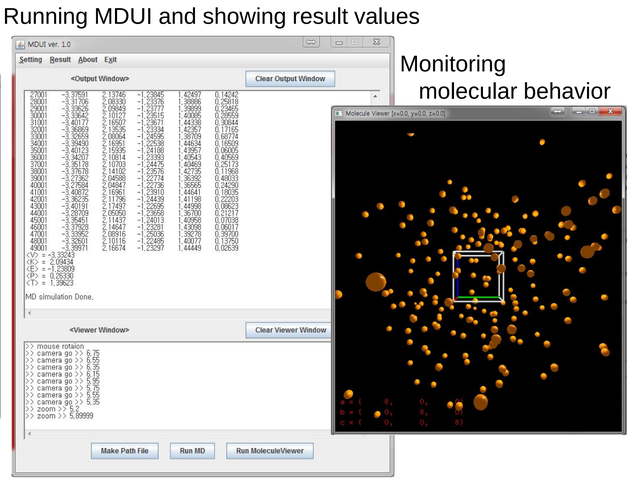
▶ Running MDUI

Run calculator and Molecule Viewer

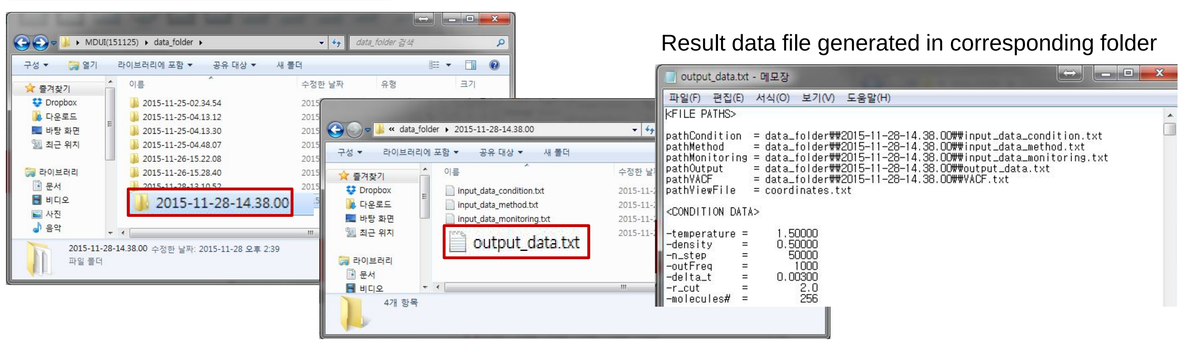


Running MDUI and showing result values

Monitoring molecular behavior



Result data file generated in corresponding folder



References

- Jaeeon Chang, Development of Molecular Simulation Software for the Prediction of Thermodynamic Properties, The Korean Institute of Chemical Engineer(2010)
- Inguk Chun and Sangho Ha, Power JAVA, INFINITY BOOKS(2014)
- M. P. Alien, D. J. Tildesley, Computer Simulation of liquids, Oxford University Press, (1987)

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