Progress on the Development of HPC Cloud Computing Platform to Support Drug Design Based on Medical Plants

Abstract

Molecular Dynamics is one part of in silico drug design processes, and it is a computer simulation method for studying the physical movements of atoms and molecules. The atoms and molecules are allowed to interact for a fixed period, giving a view of the dynamic evolution of the system*. Assuming that there are N atoms in a molecule, the time complexity is O(N2). Usually, one needs to do a great number of timesteps simulation such as in 100 Nano Second (NS) and large computing time as the number of atoms (N) are huge due to the complexity of the molecule. For example, the Gromacs results in 90 NS which shows the development of veskel DPPC (dipalmitoyl phosphatidyl choline) [De Vries2008], required 3750 days of single CPU processes, or 117,2 days of 32 CPUs processes. It is becoming more challenges as not many Research institution own HPC infrastructure, and many of the users are not in Computer Science background. In this talk, the authors will present their experience in developing a feasible Cloud Computing environment for users in developing countries, such as Indonesia. Some findings on the computing aspects and some results on Indonesia medical plants simulation will be given.

*[https://en.wikipedia.org/wiki/Molecular_dynamics]