Performance Analysis of Molecular Dynamics Simulation of PfENR Enzyme using AMBER on Cluster and GPU computing environment

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ABSTRACT
One of the processes requiring HPC environments is Molecular Dynamics (MD) . In tropical countries, the MD process is very important in the preparation of virtual screening experiments for anti-malaria search. Previous works on the virtual screening project for anti-malaria search conducted by WISDOM project uses grid infrastructure with 1,700 CPUs of various infrastructure provided in 15 countries [13]. In silico anti malaria compounds searching from Indonesian medical plants using virtual screening methods are urgently required. This can reduce the cost and time required compared to the direct searching or examining each compound by in vitro and in vivo which will spend a lot of time and expense . However, the use of thousands of processors is difficult for the researchers with limited resources in developing countries such as Indonesia.
Our of previous studies using MD with GROMACS shows the improvement of the simulation time using Cluster. But that is not the case for some of our previous works with AMBER on Cluster where we did not obtain significant speed up. However, our previous works running GROMACS on GPUs provided significant speed up about 12 times faster than that run on Cluster. In this study , we build a GPU -based computing environment and have some MD simulation with AMBER.
We used several computing environments such as cluster with 16 cores , GPU Geforce GTX 465 , GTX 470 , GTX 560 , GTX 680 , and GTX 780 . In addition to PfENR (Plasmodium falciparum Enoyl acyl Carrier Protein Reductase) enzyme , as benchmark we also conducted MD experiments on Myoglobin protein , Dihydrofolate reductase (DHFR) protein, and Ras - Raf protein . All experimental results showed that the slowest MD processes occurred on Cluster, followed in increasing order by GTX 560, GTX 465, GTX 470, GTX 680 and GTX 780. While the GPU speed up relative to cluster is about 24 , 26 , 32 , 24 , 77 and 101, respectively.