Using Dedicated and Non Dedicated HPC Cluster and GPU NVIDIA Tesla C2070 Cloud computing environment to simulate Molecular Dynamics of PfENR Enzyme with AMBER

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ABSTRACT
Molecular Dynamics (MD) is one of processes that requires High Performance Computing environments to complete its jobs. In the preparation of virtual screening experiments, MD is one of the important processes particularly for tropical countries in searching for anti-Malaria drugs. The search for anti-Malaria has previously conducted, for example by WISDOM project utilizing 1,700 CPUS. This computing infrastructure will be one of the limitation for country like Indonesia that also needs in silico anti malaria compounds searching from the country medical plants. Thus finding suitable and affordable computing environment is very important. Our previous works showed that our dedicated Cluster computing power with 16 cores performance better than those using fewer cores, however the GPU GTX family computing power is much better.
In this study, we investigate further our previous experiment in finding more suitable computing environment on much better hardware specification of non dedicated Cluster computing and GPU Tesla. We used two computing environments, the first one is Barrine HPC Cluster of The University of Queensland which has 384 compute nodes with 3144 computing cores. The second one is Delta Future Grid GPU Cluster which has 16 computing nodes with 192 computing cores, each nodes equipped with 2 NVIDIA Tesla C2070 GPU (448 cores). The results show that running the experiment on a dedicated computing power is much better than that on non dedicated ones, and the GPU performance is still much better than that of Cluster.