# The performance of a molecular dynamics simulation for the plasmodium falciparum enoyl-acyl carrier-protein reductase enzyme using amber and gtx 780 and 970 double graphical processing units

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Abstrak

The invention of graphical processing units (GPUs) has significantly improved the speed of long processes used in molecular dynamics (MD) to search for drug candidates to treat diseases, such as malaria. Previous work using a single GTX GPU showed considerable improvement compared to GPUs run in a cluster environment. In the current work, AMBER and dual GTX 780 and 970 GPUs were used to run an MD simulation on the Plasmodium falciparum enoyl-acyl carrier protein reductase enzyme; the results showed that performance was improved, particularly for molecules with a large number of atoms using single GPU.