Design and Analysis GPU Computing for Molecular Dynamics Simulations with AMBER Applications

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Problems

- Molecular Dynamics (MD) is one of the important processes in drug design research
- MD simulation requires high performance computing resources
- Computing resource is one of the limitation for a researchers in performing MD simulations to support research in drug discovery process based on Indonesia medical plants.
- 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.

Solutions Suggested

Building and finding suitable and affordable computing environment for Molecular Dynamics research by utilizing:

- Dedicated computing environment with single and multi GPU
- Public cloud computing Delta Future Grid and Stampede XSEDE.
- Optimizing MD Simulation software (AMBER) on GPU

Methodology

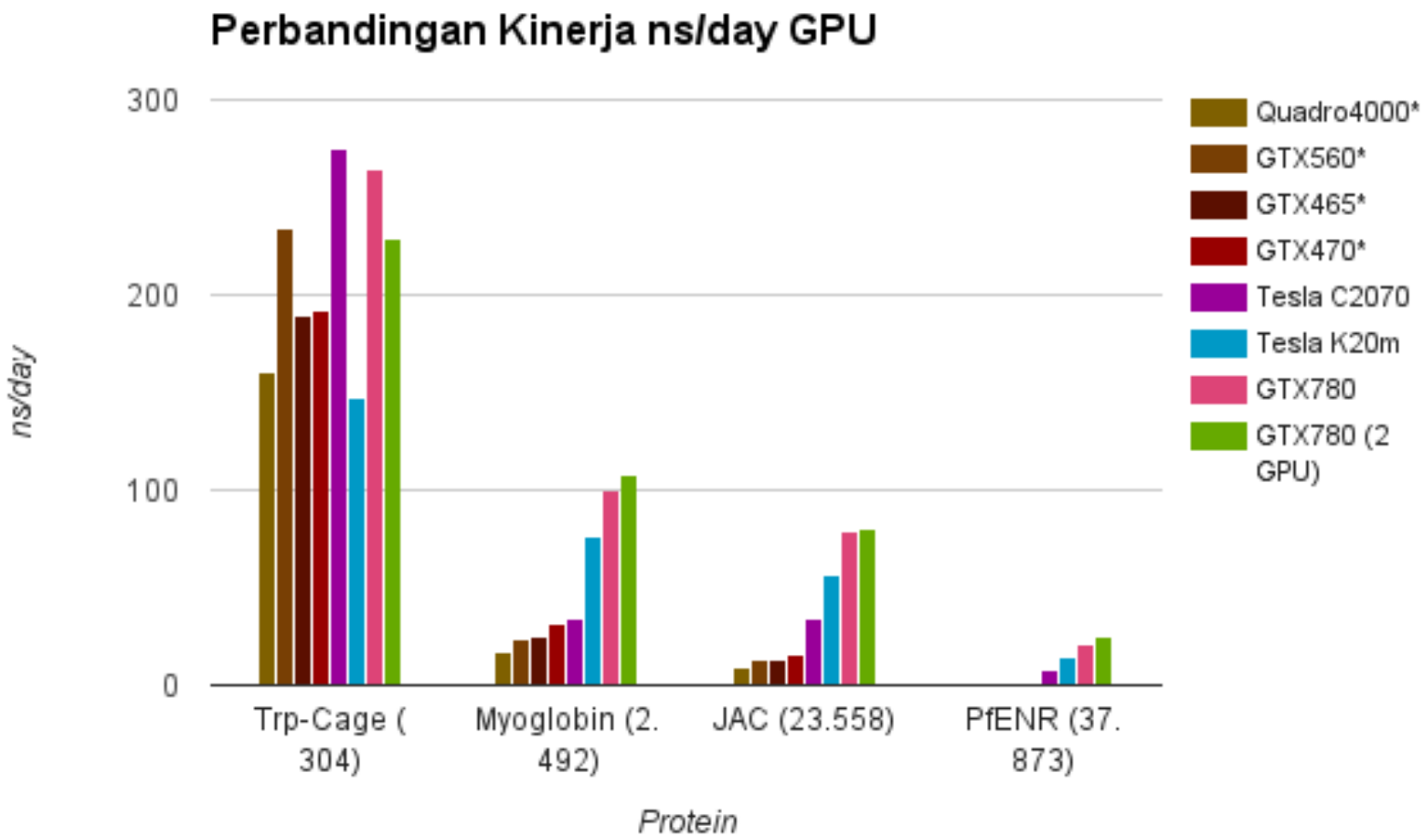
Preparation

- GPU computing environment:
  - Komputer Riset 970 (Dedicated GPU Computing): 2x NVIDIA Gforce GTX 780, Intel(R)Core i7 4 GHz, 32 GB Memory, Debian 3.2
  - Delta Future Grid[1] (Public Cloud Computing): 2x NVIDIA Tesla C2070, Intel X5560 2.8GHz, 192GB Memory, Red Hat Linux
  - Stampede XSEDE[2] (Public Cloud Computing): NVIDIA Kepler 2, Intel Xeon E5-2680, 200TB Memory, CentOS Linux
- Software:
  - CUDA 5, CUDA Toolkit, AMBER12, Optimizing parameters (adjusted with suitable grid size and the number of threads)
- Protein:
  - PfENR (N atom 37.873), JAC (N atom 23.558), TRPCage (N atom 304), Myoglogin (N atom 2.492), Nucleosome (N atom 25.095)

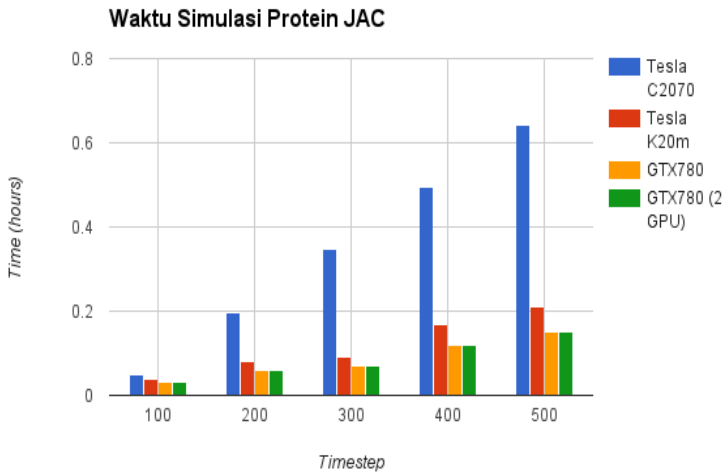
[1] http://futuregrid.org

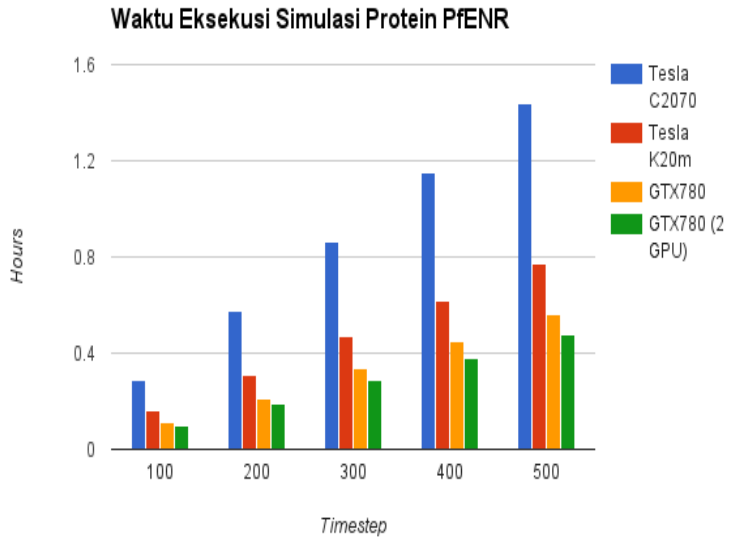
[2] https://portal.xsede.org/tacc-stampede

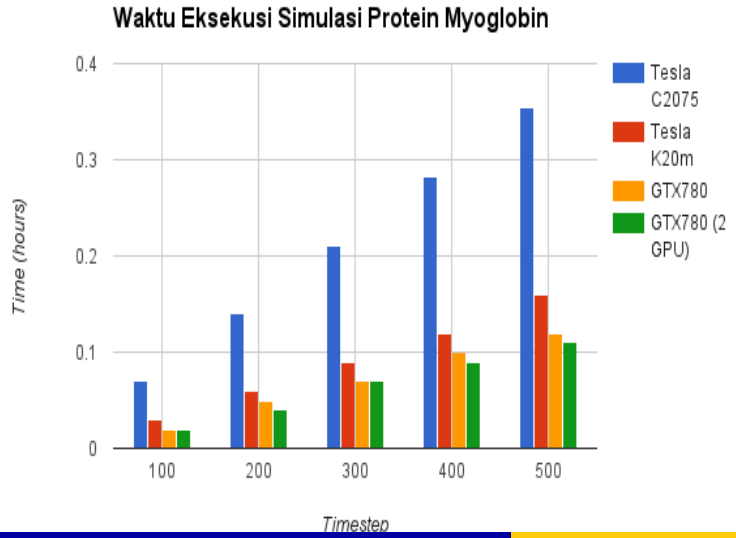
Result: NS/day

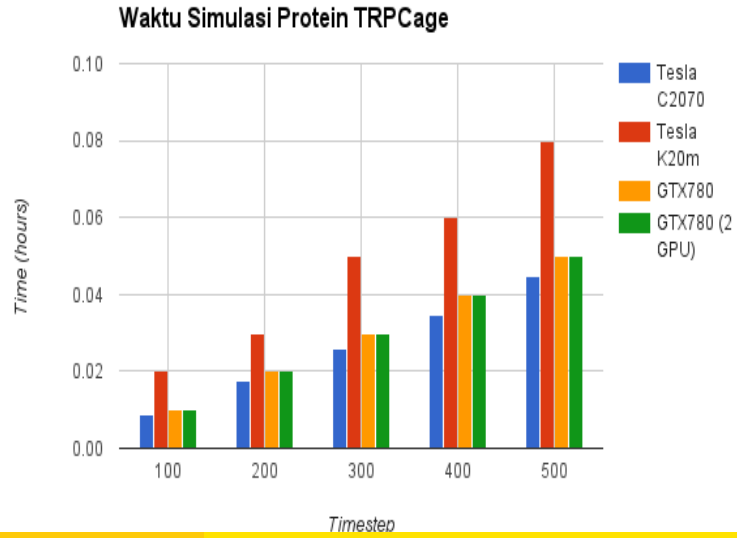


Result: Simulation Time

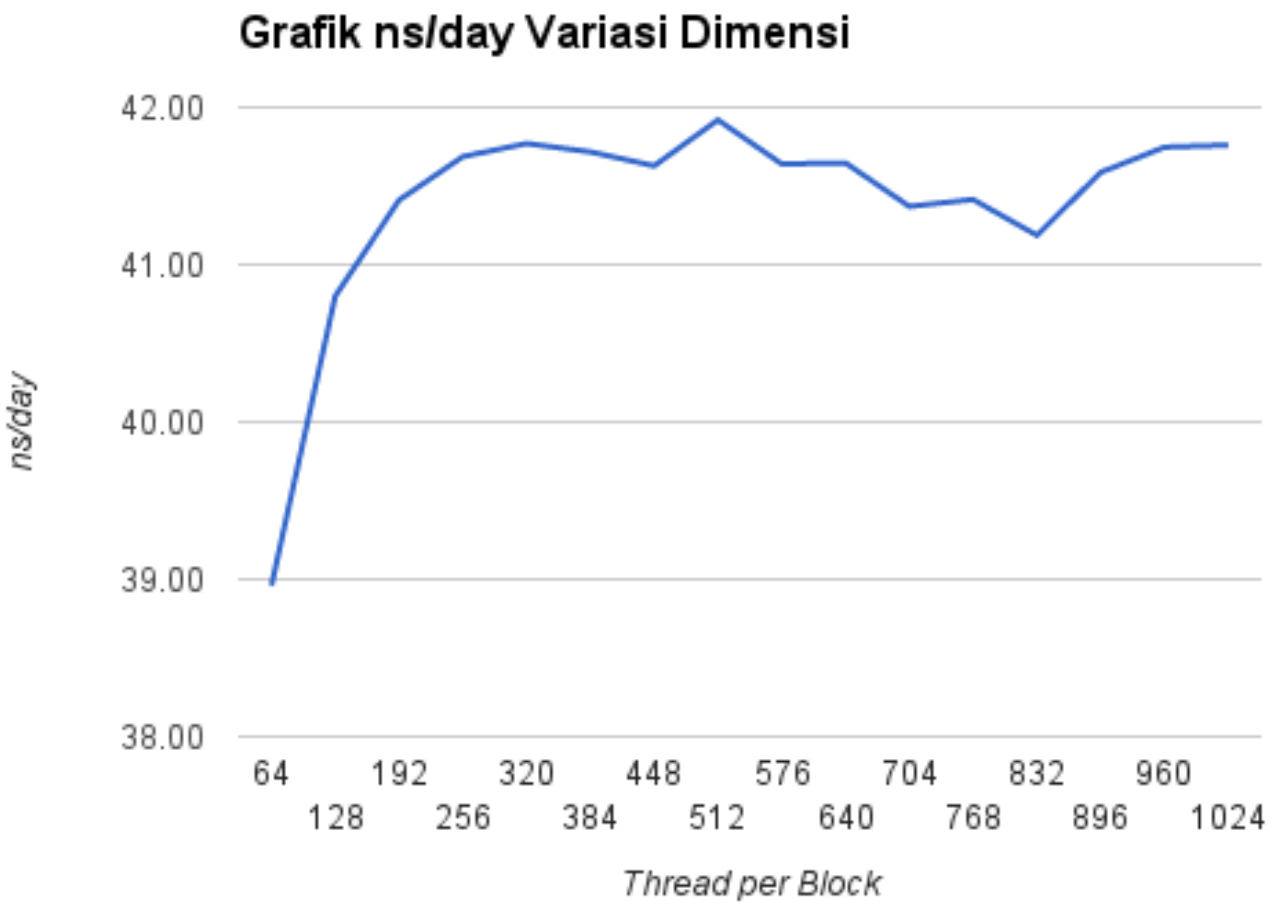




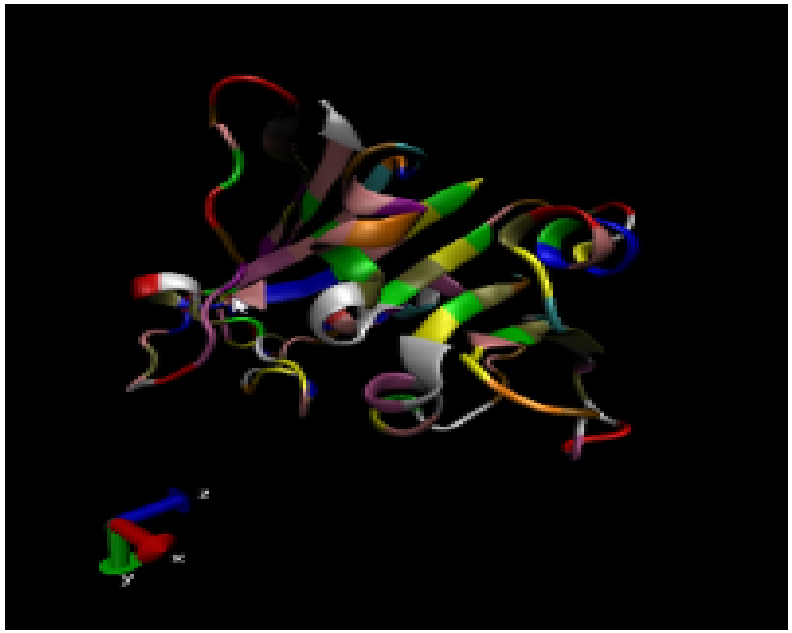


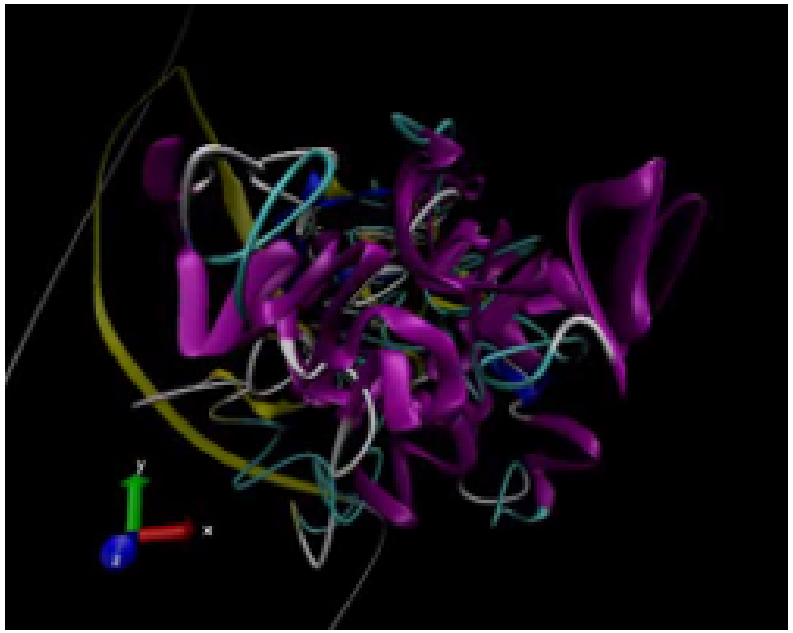


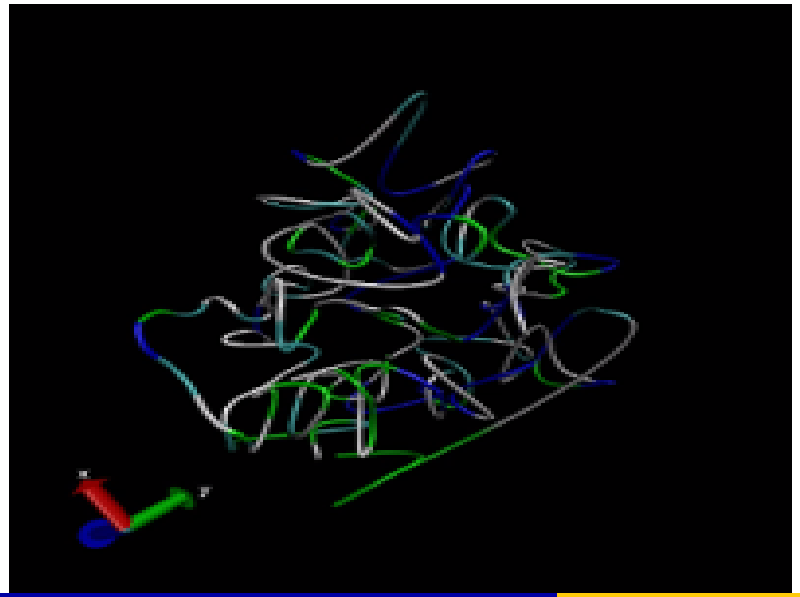
Result: Optimizing Parameter

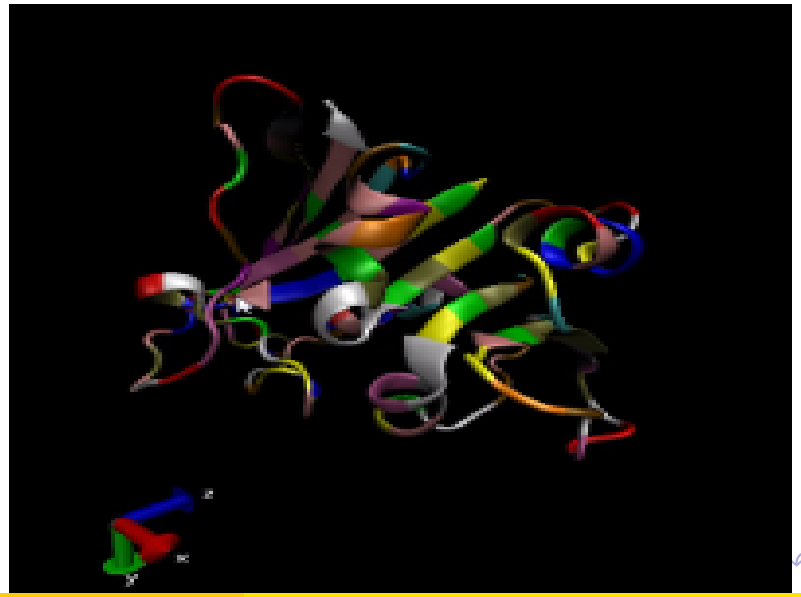


Result









Conclusion and Future work

- Conclusion
  - Public cloud computing can be a solution for a molecular dynamic simulations resource computing problem.
  - The result is determined by the GPU spesifications both on public and dedicated computing environment. The much better hardware specification providing much better performance.
  - The use of public computing environment has an waiting times but may be considered in terms of convenience.
  - MD simulation performance increase with using multiGPU for large-sized proteins.
- Future Work
  - Next experiment using new version AMBER (AMBER14) for support multiGPU scalling
  - Experiment on commercial public cloud computing (ex: Amazon EC2, Azzure, dll) to calculate the cost of MD simulation

Thank you
Terima kasih