NAMD Benchmarking on Publicly Available Philippine Computational Resources

Ronny L. Cheng†, Ren Tristan A. dela Cruz †,‡, Francoise Neil D. Dacanay †, Gil C. Claudio † and Ricky B. Nellas †

† Institute of Chemistry, University of the Philippines, Diliman, Quezon City
‡ Department of Computer Science, University of the Philippines, Diliman, Quezon City
Molecular dynamics allows us to study molecular interactions leading to potentially new discoveries.

Drug Design

Protein Engineering

Materials Science

Taken from http://www.cadd.ethz.ch/research/polypharmacology/_jcr_content/image.imageformat.carousel.1348723969.png, http://www.codata.org/uploads/images/nano_image01.png and https://static.wixstatic.com/media/85df7b_ed9efc9e1e7140539a0a3479344dbcd9.png/v1/fill/w_371,h_208,al_c,usm_0.66_1.00_0.01/85df7b_ed9efc9e1e7140539a0a3479344dbcd9.png
Use of high performance computing in Molecular Dynamics

- MD simulations are computationally expensive
- GPUs now used in tandem with CPUs to increase computing capabilities
- GPU-accelerated desktops now being used as cost-effective alternatives to HPCs

Taken from Wageningen University and Research. “Molecular Dynamics: internal dynamics of an IgG Domain.”
What is NAMD?

- Uses parallel processors to handle MD of large molecules
- **Scalable**
- Is already capable of simulating up to 2.64 million atoms in the femtosecond scale
- NAMD performance related to:
  - system size
  - number of parallel processors
  - Intercommunication infrastructure
Different time-scales show different types of protein interactions

Taken from “Jung, J. (2015) “Parallelization of molecular dynamics.” Presented at CMSI計算科学技术特論 A.”
Objectives

• Benchmark NAMD using different publicly available computer resources located in the Philippines
• Use results to determine how long to complete an MD simulation of a specific size
• Use results to create a Philippine roadmap for development of biomolecular computations and related researches
Systems and Methods

- **Identify systems**
- **Set-up systems**
- **Set-up MD conditions**
- **Run MD simulations**

**Small system size** (~10,000 atoms)
- Anoplin
- Kalata B1 (1NB1)

**Medium system size** (~20,000 atoms)
- Pseudomonas aeruginosa lipase (1EX9)

**Large system size** (>50,000 atoms)
- N. Atlantic ocean pout antifreeze (1KDF)
- Octopamine receptor in mushroom bodies (OAMB)
Systems and Methods

4 computing resources:

1) ASTI HPC (48 × Intel Xeon CPU E5-2697 v2 @ 2.70 GHz)

2) BlueGene/P (1 rack, 1024 × 4-core IBM PowerPC 450 @ 850 MHz)

3) CSRC HPC (2 × 4-core Intel Xeon CPU E5405 @ 2.0 GHz)

4) GPU-accelerated High-end desktop (4 × Intel Core i7-4790 with 4 virtual cores @ 3.60 GHz accelerated with NVIDIA GeForce Jetstream GTX970)
Results: ASTI HPC performance

- Can simulate ~4.58 ns/day for OAMB and ~32.98 ns/day for anoplin
- Scaling breakdown can be attributed to high latency of Gigabit Ethernet network
- Advantage: accessibility
- Disadvantage: interference due to multiple jobs
Results: BlueGene/P performance

- Can simulate \( \sim 6.05 \) ns/day for OAMB and \( \sim 30.03 \) ns/day for anoplin
- NAMD scalable using BlueGene/P
- Parallel efficiency not maximized yet
- Reduced latency due to 3D torus intercommunication network
  - Reduced latency \( \rightarrow \) less intercommunication time
Results: CSRC HPC performance

- Can simulate between ~ 0.95 ns/day for OAMB and ~ 11.19 ns/day for anoplin
- Processor capability as bottleneck
Results: high-end desktop performance

- Simulates between $\sim 4.05$ ns/day for OAMB and $\sim 44.64$ ns/day for anoplin
- Scaling breakdown after 4 processors
- Hyperthreading was not beneficial
  - SDRAM component (DDR3 was used)
- Poor scalability of NAMD in high-end desktop
Comparison: anoplin as a small system size

- In terms of ns/day: high-end desktop > ASTI > BlueGene/P > CSRC
- Minimal dependence on intercommunication
- Processor speed dependent
  - High-end desktop have better computational capabilities
Comparison: 1KDF as a medium system size

- High-end desktop ≈ BlueGene/P > ASTI > CSRC
- Increased importance of inter-communication
Comparison: OAMB as a large system size

- BlueGene/P > high-end desktop > ASTI > CSRC
- Intercommunication as the vital factor
- Further speed-up can be done by increasing processors in CSRC HPC, ASTI HPC and BlueGene/P
Conclusion

- Increased system size leads to decreased ns/day generated
- High end desktop generated the most ns/day for small and medium system sizes
- BlueGene/P is recommended for larger system sizes
- However, generated ns/day lags in comparison to international counterparts
References


Images:

http://www.cadd.ethz.ch/research/polypharmacology/_jcr_content/image.imageformat.carousel.1348723969.png

http://www.codata.org/uploads/images/nano_image01.png

https://static.wixstatic.com/media/85df7b_ed9efc9e1e7140539a0a3479344dbcd9.png/v1/fill/w_371,h_208,al_c,usm_0.66_1.00_0.01/85df7b_ed9efc9e1e7140539a0a3479344dbcd9.png