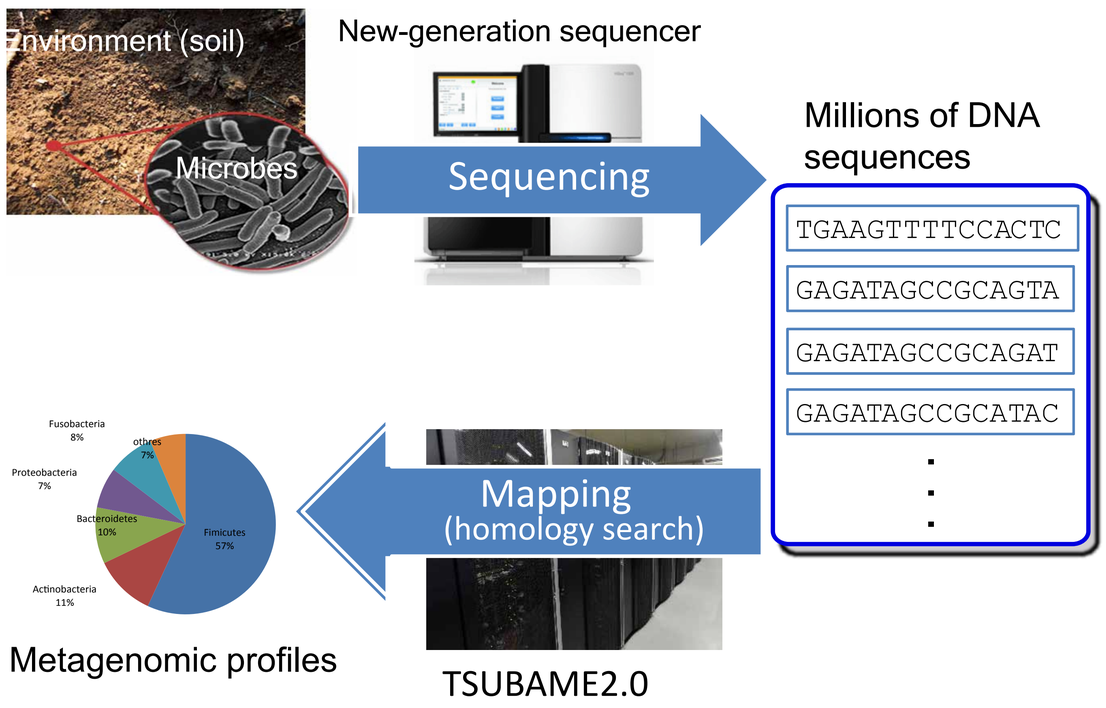
Biological Supercomputing Applications

TOKYO TECH Pursuing Excellence

Ultra-fast pipeline for metagenomics

Metagenome analysis:

The study of the genomes of uncultured microbes obtained directly from microbial communities in their natural habitats such as soils, seas, and human bodies.

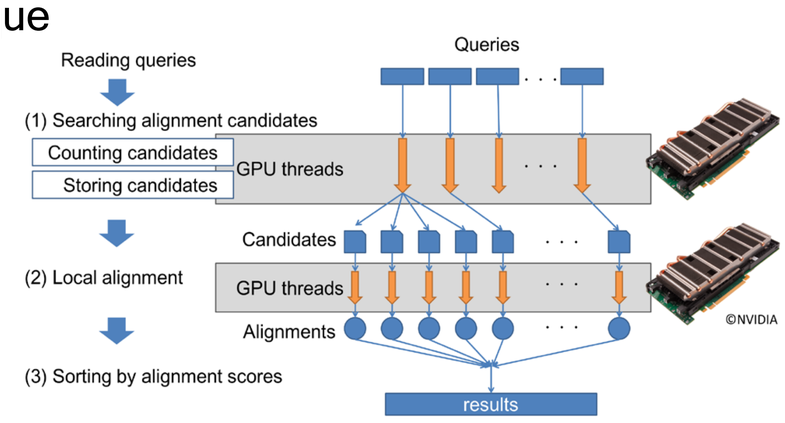


Requires massive computing power to annotate huge amout of DNA sequences obtained from new generation sequencers (NGSs)

Contact: Yutaka Akiyama (Tokyo Tech)

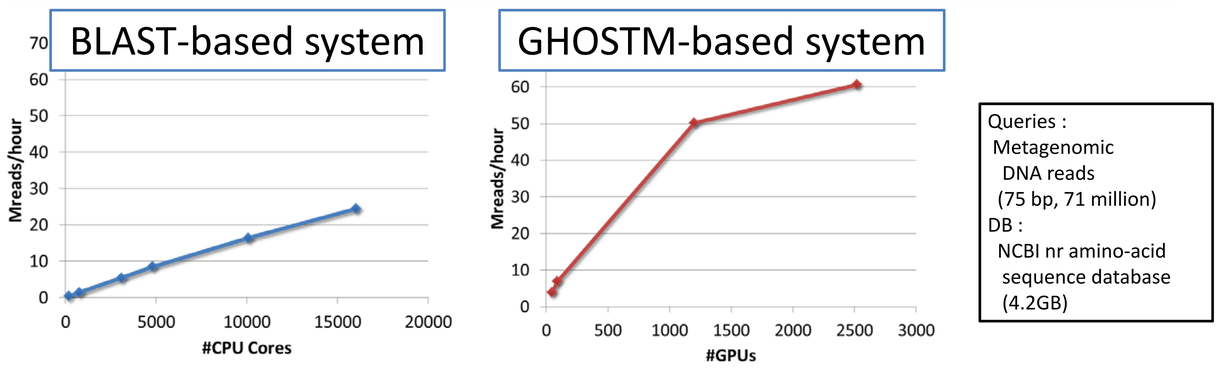
GHOSTM: GPU-based fast homology search tool

130 times faster than BLASTX by using GPU-computing technique



[1] Suzuki, S., Ishida, T., Kurokawa, K. and Akiyama, Y. 2012. GHOSTM: A GPU-Accelerated Homology Search Tool for Metagenomics. ***PLoS ONE***. 7, 5, e36060.

Automated pipeline on TSUBAME 2.0



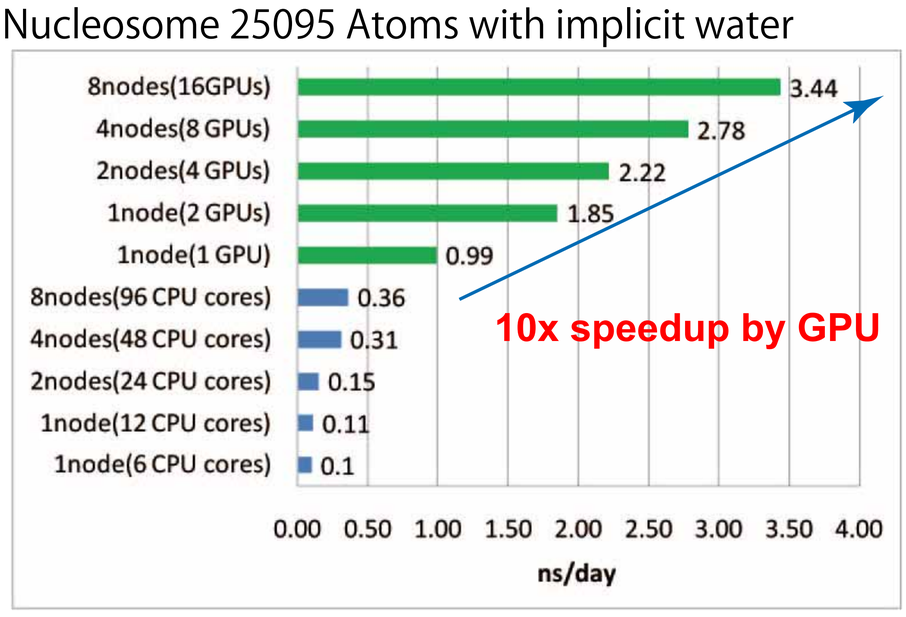
The pipeline achieved to process

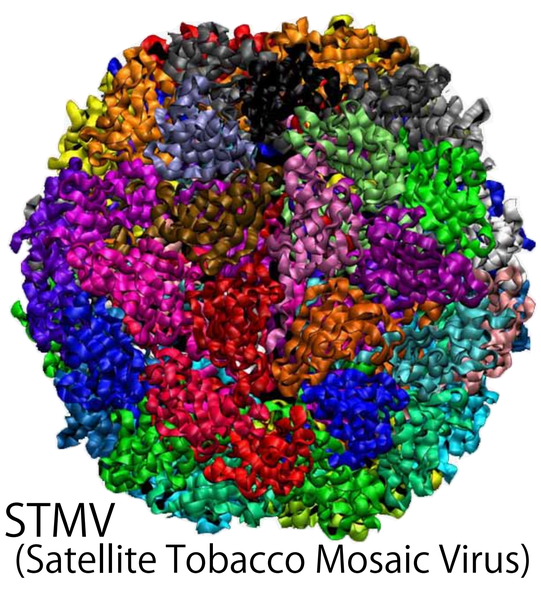
- about 24 million reads per an hour with 16,008 CPU cores
  (the BLASTX-based system , 1,334 computing nodes)
- about 60 million reads per an hour with 2,520 GPUs
  (the GHOSTM-based system, 840 computing nodes)

Accelerating MD simulation

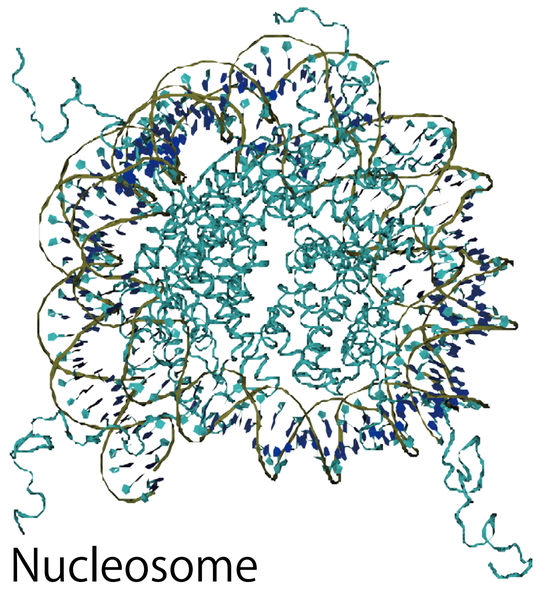
Molecular Dynamics (MD) is a simulation method that track the motion of atoms based on classical mechanics. We executed performance evaluations of MD applications, AMBER11[1] and NAMD2.8[2], on TSUBAME2.0.

Amber11 PMEMD Performance:
Nucleosome 25095 Atoms with implicit water



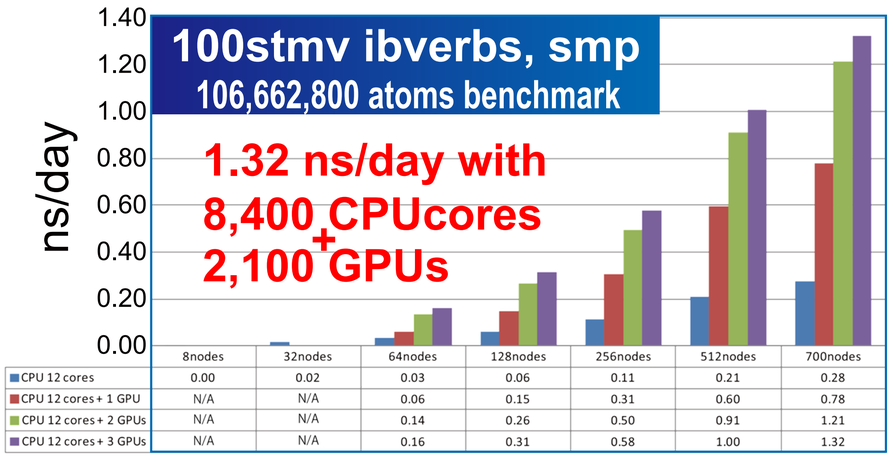


STMV
(Satellite Tobacco Mosaic Virus)



Nucleosome

NAMD 2.8 Performance:
100x STMV 106,662,800 atoms including water



	8nodes	32nodes	64nodes	128nodes	256nodes	512nodes	700nodes
CPU 12 cores	0.00	0.02	0.03	0.06	0.11	0.21	0.28
CPU 12 cores + 1 GPU	N/A	N/A	0.06	0.15	0.31	0.60	0.78
CPU 12 cores + 2 GPUs	N/A	N/A	0.14	0.26	0.50	0.91	1.21
CPU 12 cores + 3 GPUs	N/A	N/A	0.16	0.31	0.58	1.00	1.32

[1]D.A. Case et al. (2010), AMBER 11, University of California, San Francisco.
[2]James C. Phillips et al. Scalable molecular dynamics with NAMD. Journal of Computational Chemistry, 26:1781-1802, 2005.

Contact: Masakazu Sekijima (Tokyo Tech)

http://www.gsic.titech.ac.jp/sc12