UbuntuNet CONNECT 2014

Cloud-Based Big Data Analytics in Bioinformatics

Presented

By

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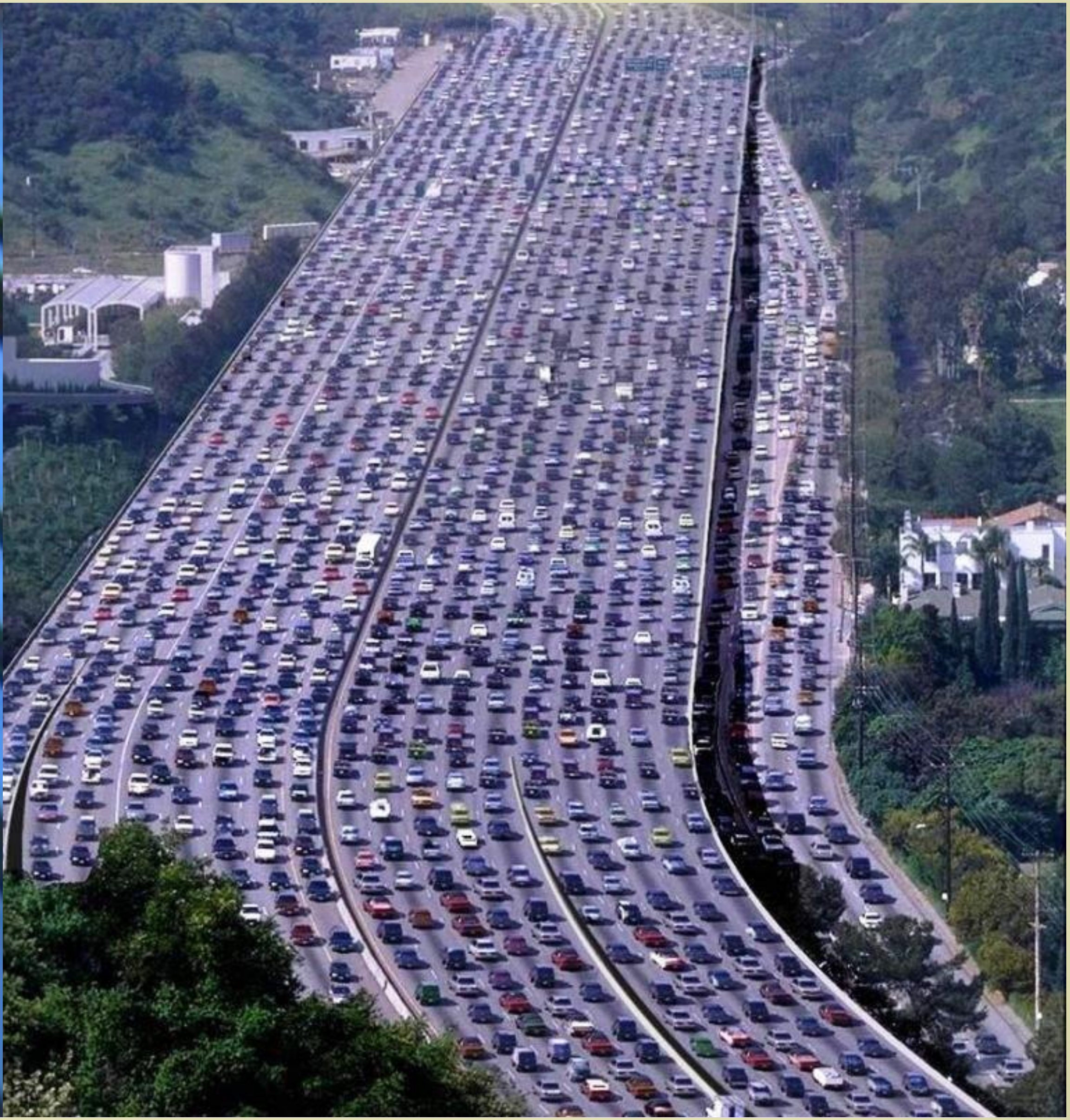
success through innovation

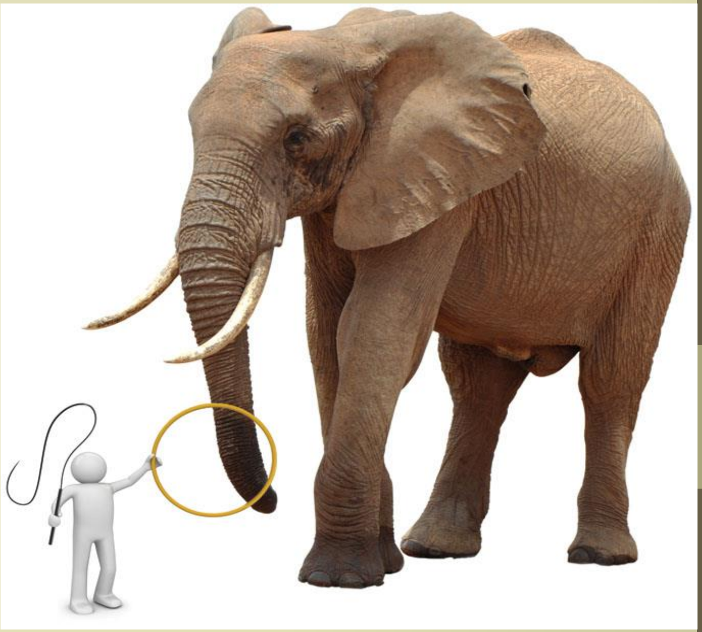
Introduction



Big Data Analytics

- **Big Data** are a collection of data sets so large and complex that it becomes difficult to process using on-hand database management tools or traditional data processing applications.
- The process of research into massive amounts of such data to reveal hidden patterns and secret correlations is thus called **big data analytics**.

❑ High-throughput technologies in bioinformatics



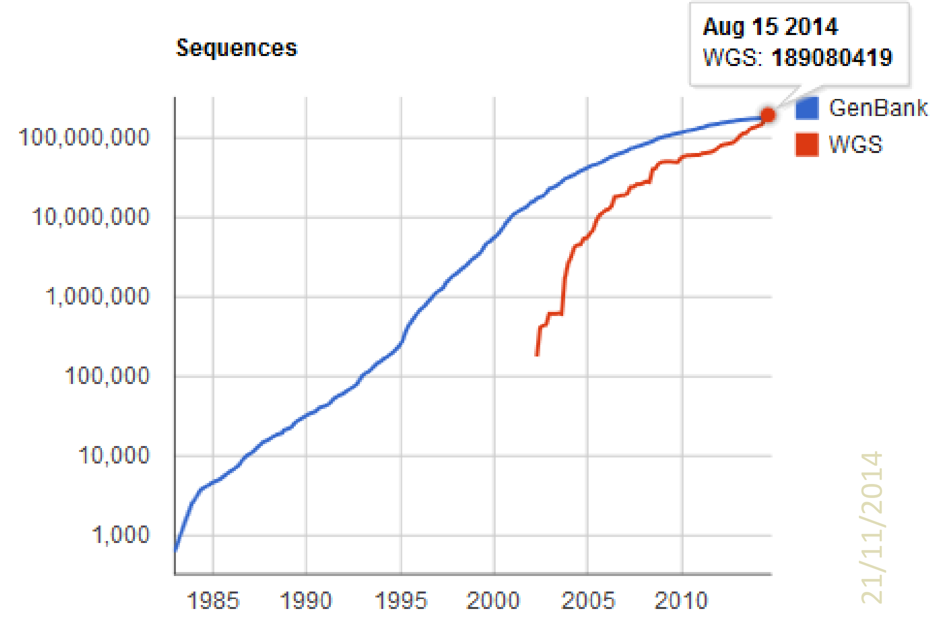
High-throughput Technologies

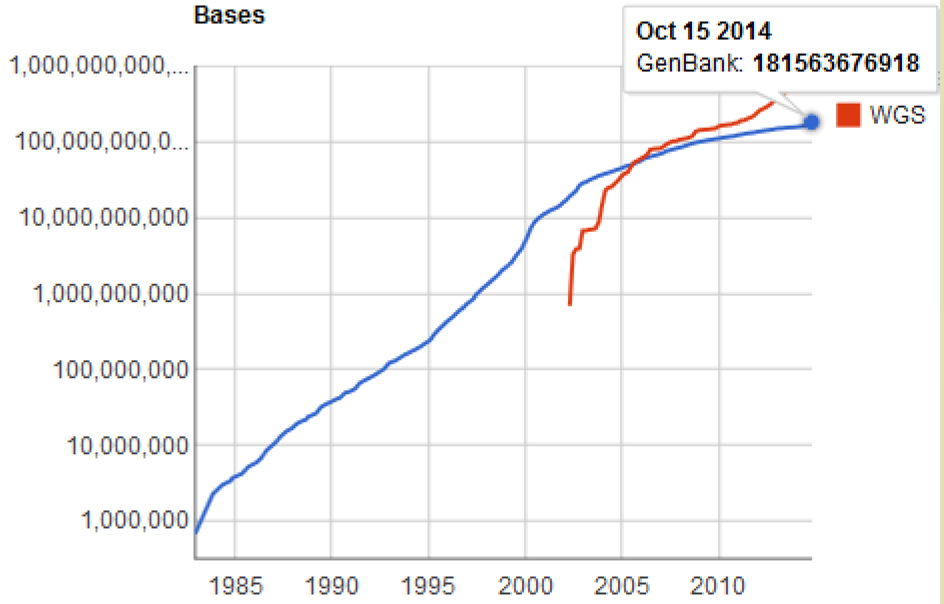
- Next Generation Sequencing (NGS)
- Virtual Screening
- Genotyping
- SNP (Single Nucleotide Polymorphism) discovery
- Gene expression
- Proteomics

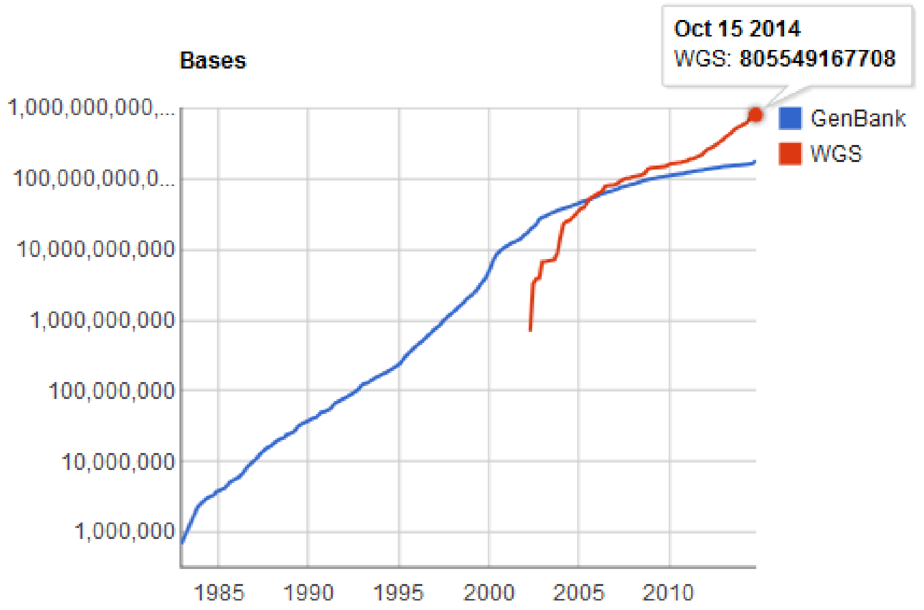
- ➢ Sequence mapping
- ➢ Sequence analysis
- ➢ Peak caller for ChIP-seq data
- ➢ Identification of epistatic interactions of SNPs
- ➢ Drug discovery

- ❖ Data storage
- ❖ Data complexity
- ❖ Memory management
- ❖ Computational power

Example: Next Generation Sequencing (NGS)….ACGTACCT







http://www.ncbi.nlm.nih.gov/genbank/statistics. Accessed on Oct 21, 2014

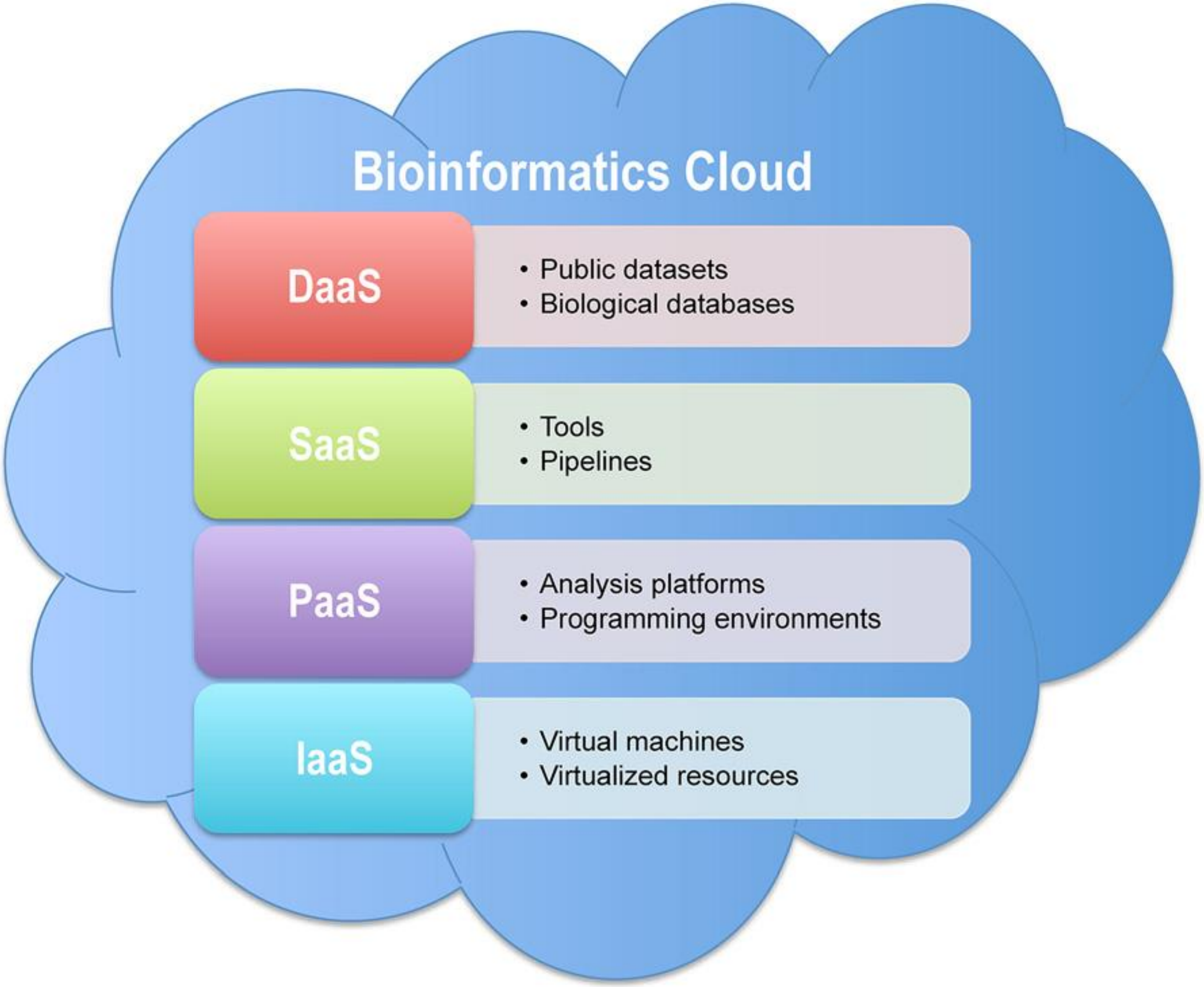
What Next?

Cloud Computing

- “computing in which dynamically scalable and virtualized resources are provided as a service over the internet”.

- ✓ Unified, location- independent platform for data & computation
- ✓ Pay-per-use & available even to small labs
- ✓ Affordable costs
- ✓ Linear scaling with parallel execution
- ✓ Time effective; large no. of nodes
- ✓ Up-to-date

[Bateman, A. & Wood, M. Bioinformatics 25, 1475 (2009).]



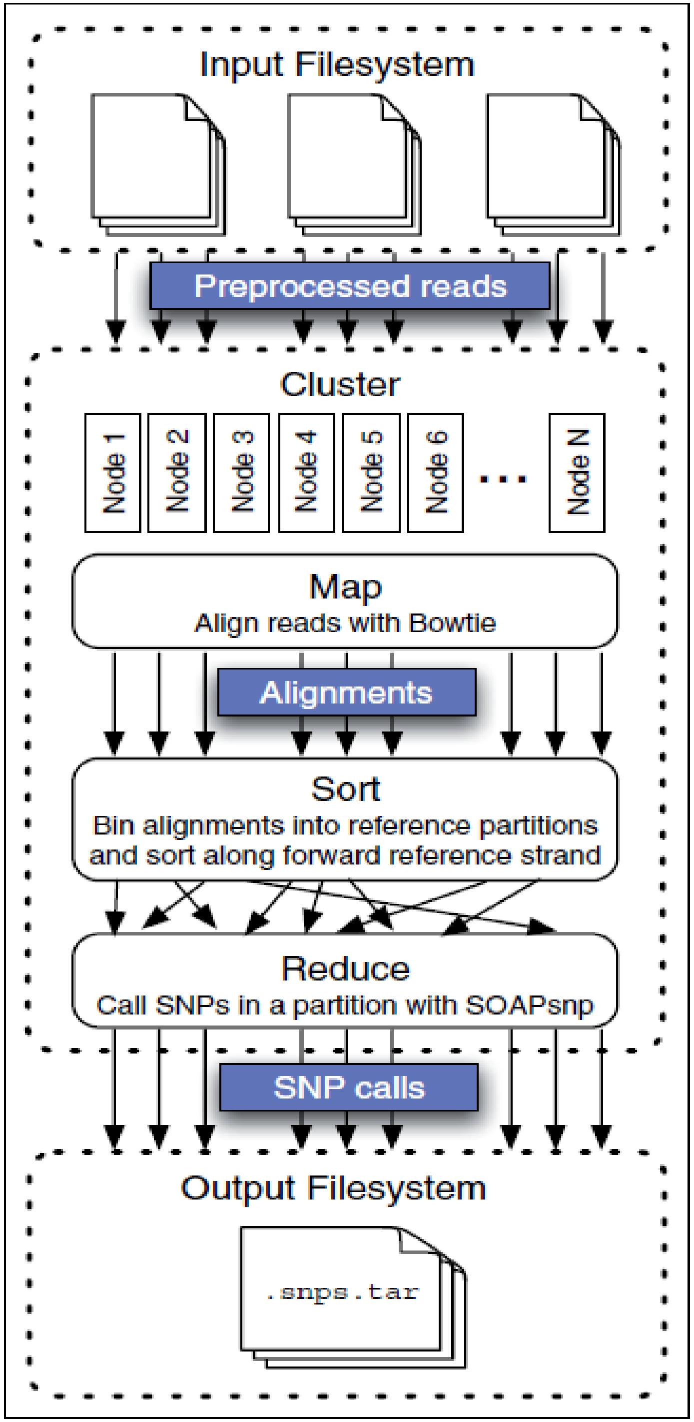
Bioinformatics Cloud

DaaS	Public datasets Biological databases
SaaS	Tools Pipelines
PaaS	Analysis platforms Programming environments
IaaS	Virtual machines Virtualized resources

❑ Cloud-based services in bioinformatics are grouped into Data as a Service (DaaS), Software as a Service (SaaS), Platform as a Service (PaaS), and Infrastructure as a Service (IaaS).

[Dai *et al*. Biology Direct 2012, 7:43. http://www.biology-direct.com/content/7/1/43]

Crossbow: Hadoop Streaming



Input Filesystem

Preprocessed reads

Cluster

Node 1 Node 2 Node 3 Node 4 Node 5 Node 6 … Node N

Map
Align reads with Bowtie

Alignments

Sort
Bin alignments into reference partitions and sort along forward reference strand

Reduce
Call SNPs in a partition with SOAPsnp

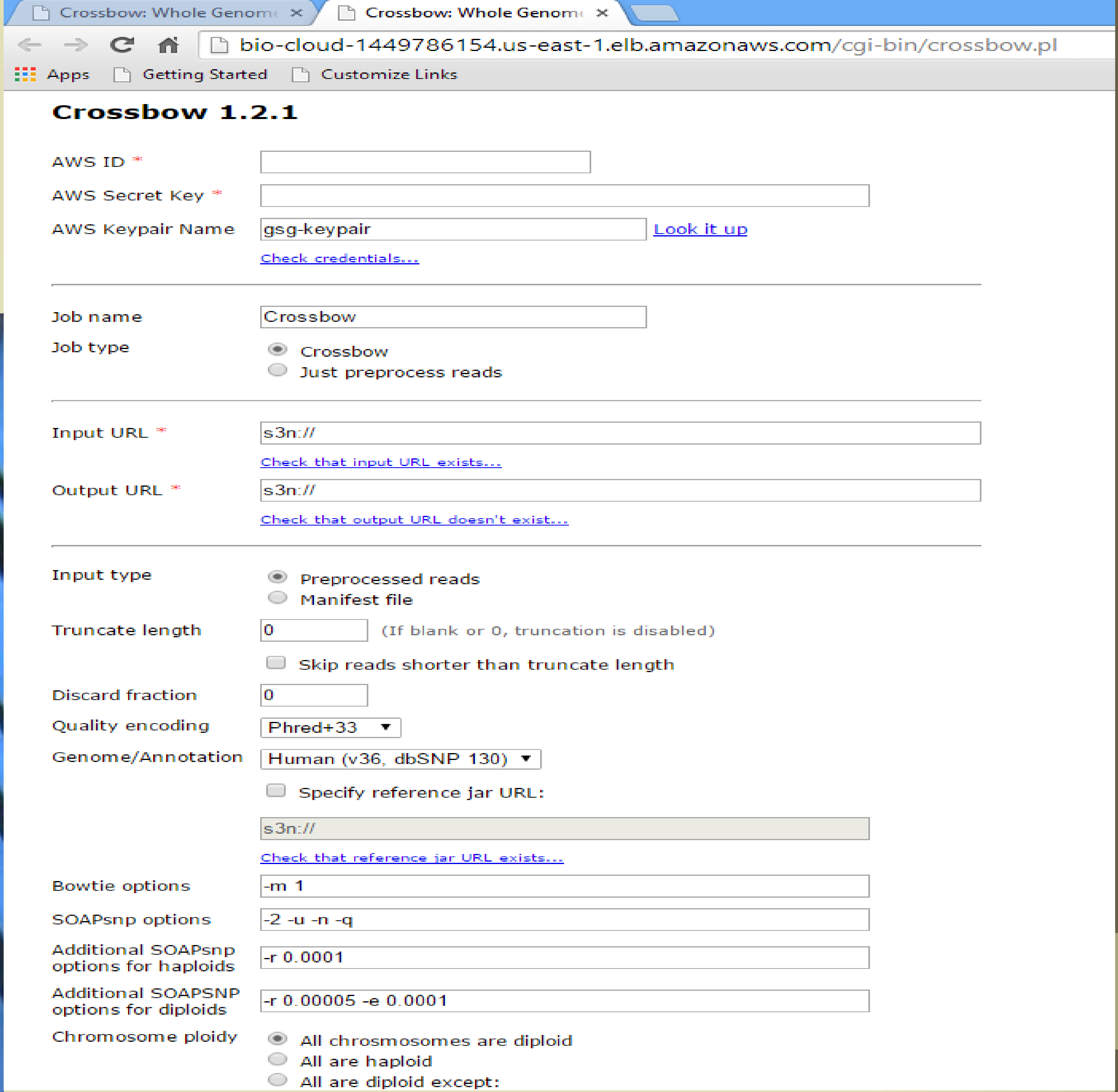
SNP calls

Output Filesystem

`.snps.tar`

Langmead, B., Schatz, M. C., Lin, J., Pop, M., & Salzberg, S. L. (2009). Searching for SNPs with cloud computing. *Genome Biol*, *10*(11), R134.

- 2.7B reads genotyped in < 3hrs on EC2 using a 320 CPU cluster for a cost of $85.



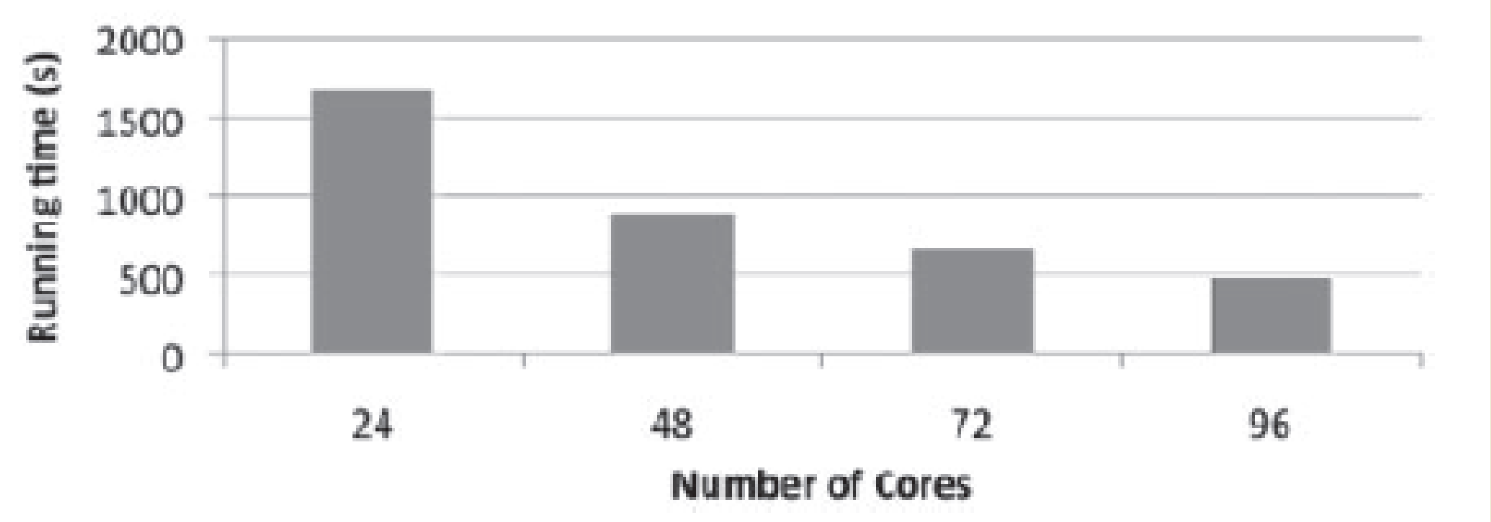
Crossbow 1.2.1

AWS ID *	
AWS Secret Key *	
AWS Keypair Name	gsg-keypair Look it up Check credentials...
Job name	Crossbow
Job type	● Crossbow ○ Just preprocess reads
Input URL *	s3n:// Check that input URL exists...
Output URL *	s3n:// Check that output URL doesn't exist...
Input type	● Preprocessed reads ○ Manifest file
Truncate length	0 (If blank or 0, truncation is disabled) ☐ Skip reads shorter than truncate length
Discard fraction	0
Quality encoding	Phred+33 ▼
Genome/Annotation	Human (v36, dbSNP 130) ▼ ☐ Specify reference jar URL: s3n:// Check that reference jar URL exists...
Bowtie options	-m 1
SOAPsnp options	-2 -u -n -q
Additional SOAPsnp options for haploids	-r 0.0001
Additional SOAPSNP options for diploids	-r 0.00005 -e 0.0001
Chromosome ploidy	● All chrosmosomes are diploid ○ All are haploid ○ All are diploid except:

Langmead, B *et. al.*, (2009). Genome Biology, vol. 10, no. 11

CloudBurst

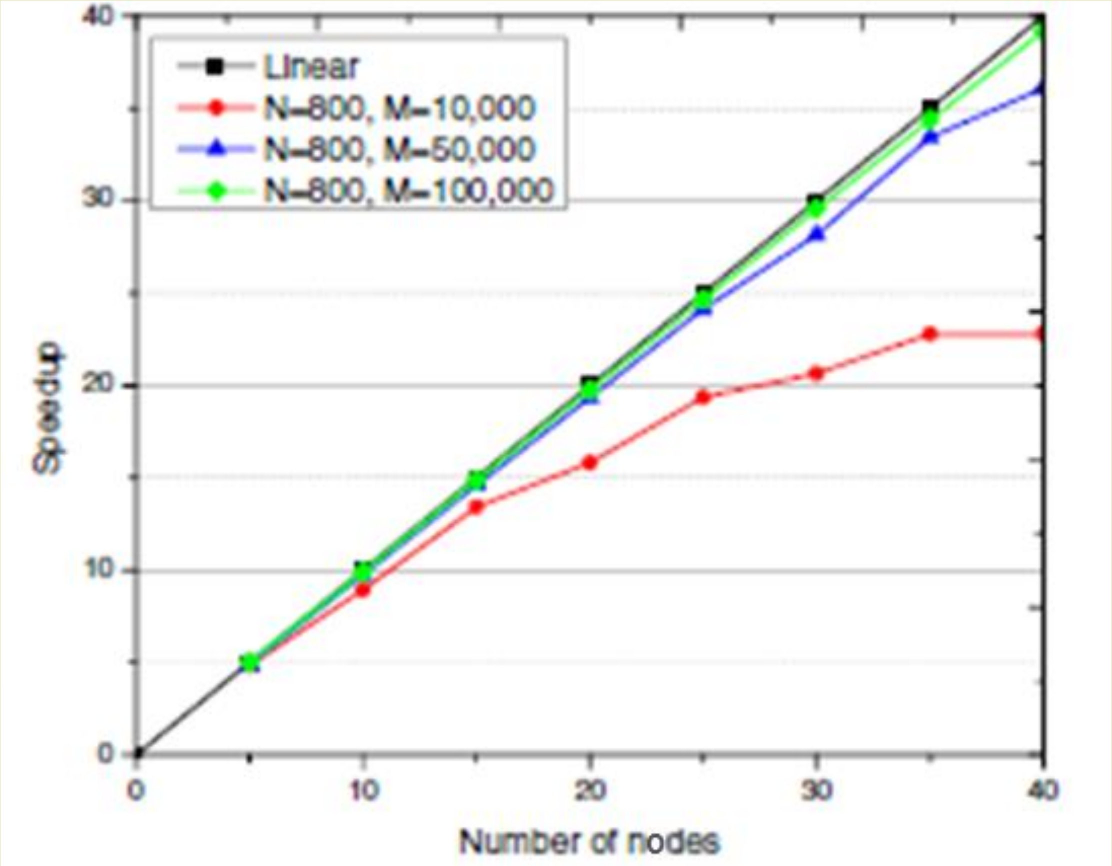
Running time on EC2 High-Medium Instance Cluster



- ☐ Comparison of CloudBurst running time while scaling the size of the cluster for mapping 7M reads to human chromosome 22 with at most four mismatches on the EC2 Cluster. The 96- core cluster is 3.5X faster than the 24- core cluster.

[Schatz. M. CloudBurst: highly sensitive read mapping with MapReduce. **Bioinformatics**, Vol.25 no. 11 2009, pp. 1363-1369.]

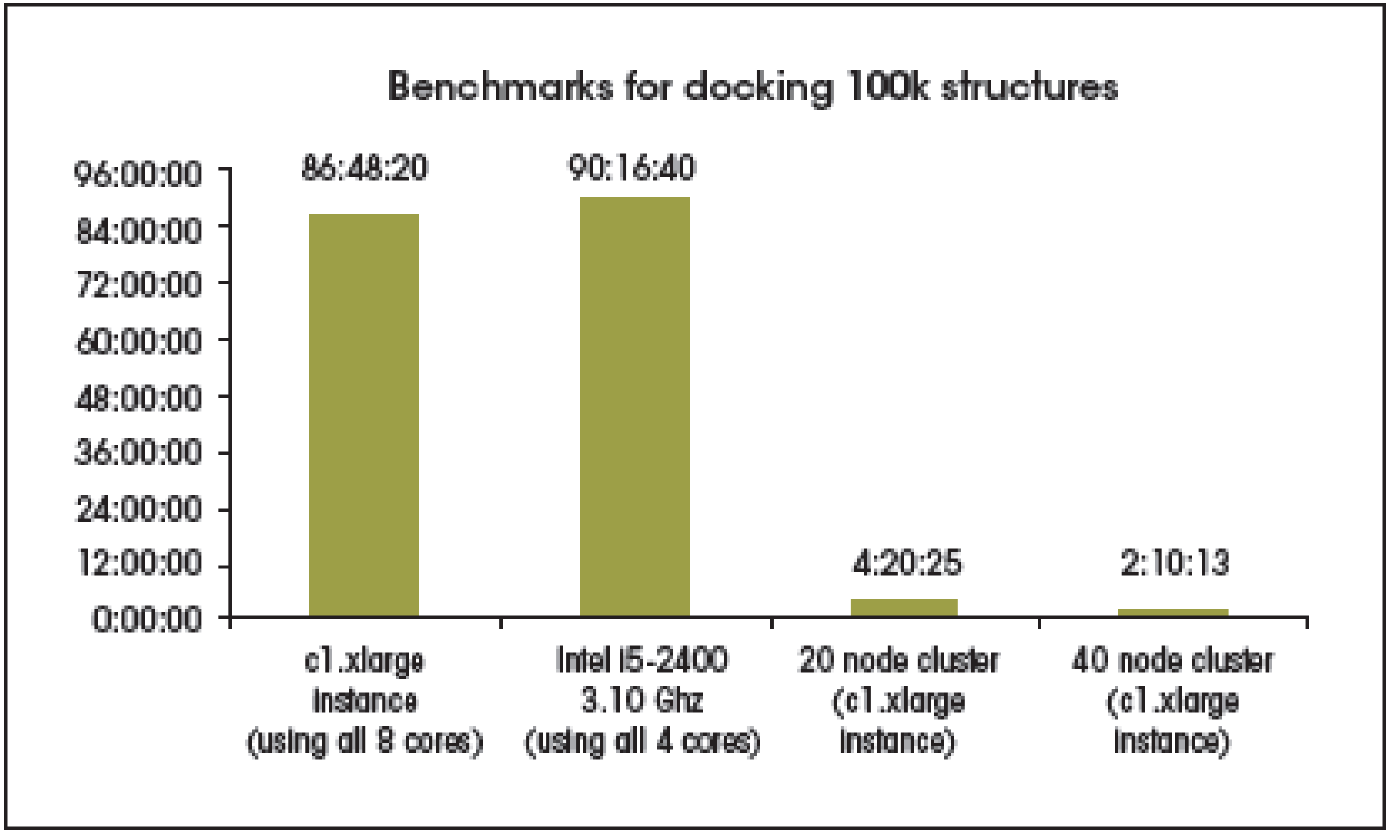
Genome-Wide Epistatic Interactions



- ❑ Computing nodes are sampled from 1-40 with 5 as interval. The red, blue, cyan and grey curve show functions of speed-up of M=10 000, M= 50 000, and M= 100 000, with size fixed to 800. # Windows Azure platform used.

Guo, X et. Al., (2014). BMC Bioinformatics 2014, **15**:102

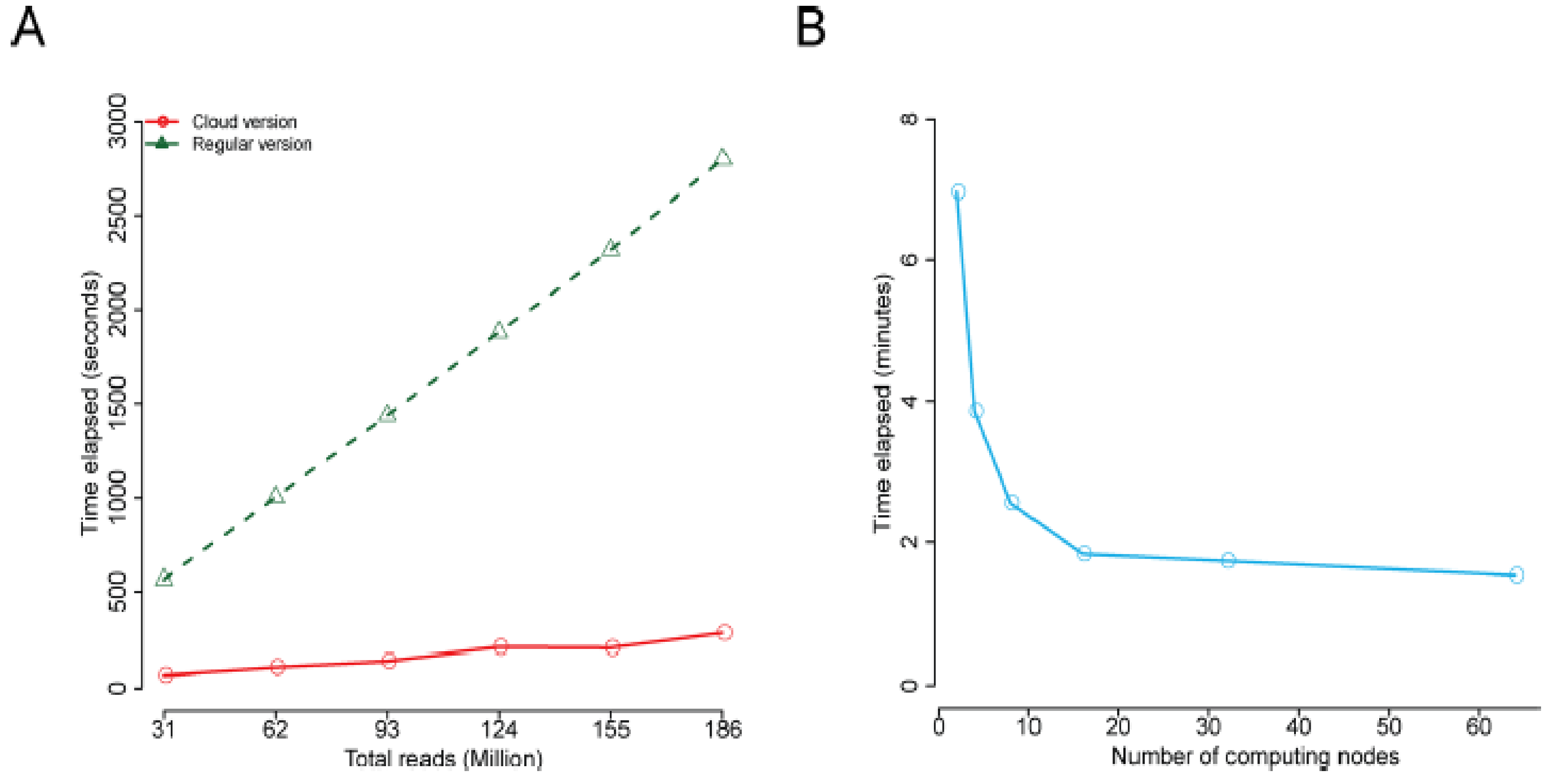
Surflex-Dock on Amazon EC2



- One C1.xlarge EC2= modern computer with 4 cores (-90hrs)
- An EC2 cluster of 40 c1.xlarge instances will thus perform in 2 hrs.
- Virtual screening (HTS) experiment for 375k ligand-receptor dockings on 160 cores was completed in < 9hrs for a total of less than $20, to find a lead in drug discovery.

www.cetara.com/cloud_computing_enables_cost_effective_virtual_screening_using_the_Amazon_cloud

PeakRanger for ChIP-seq Data



- Performance of PeakRanger in cloud parallel computing. A) test with fixed number of nodes and data sets of increasing size; B)test with increasing numbers of nodes and data sets with fixed sizes.

[Feng, X et. Al., PeakRanger: a cloud-enabled peak caller for ChIP-seq data. BMC Bioinformatics 2011, **12**:139.]

Challenges of Cloud computing

- **Security:-** trustability issues. How confidential is the data? Data is stored in a redundant manner. Limited control over remote storage.
- **Data transfer:** large data sets need to be moved to the cloud. slow upload speed. Some vendors have offered to ship data on hard drives.
- **Scalability:-** need for parallelization, and depends on the algorithm itself if MapReduce suits the use case & desired effects.
- **Usability:-** bioinformatics involves a pipeline of scripts and a command line interface. Setting up nodes in the cloud involves a lot of command line and some deeper understanding. Need for technical expertise for new apps.

Data Management

- Besides software tools that benefit the computational power and scalability of a cloud systems for data management were developed;

- Amazon hosts a lot of public datasets on their S3 storage system which are accessible for every AWS customer.

- This removes time intensive uploading processes. Same datasets can be reused by other researchers.

- Popular datasets include the annotated human genome, GenBank, HapMap or UniGene.

Conclusion & Future Work

- Cloud computing is an alternative solution to big data challenges in bioinformatics as shown by the use cases explored.
- High speed transfer technologies can be used in future to aid big data transfer
- Despite challenges still pending with data security, future efforts must be devoted to open and publicly accessible bioinformatics clouds to the whole scientific community to accelerate diagnosis, prognosis, drug discovery and personalized medicine.
- Cloud computing of big data in bioinformatics can be done on several platforms which provide a lightweight programming environment for development of pipelines.
- Bioinformatics clouds should integrate both data and software tools

Thank You

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