USING HPC CLASS INFRASTRUCTURE FOR HIGH THROUGHPUT COMPUTING IN GENOMICS

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FUNDAMENTAL RESEARCH DIVISION
GENOMIC INSTITUTE
SCIENTIFIC COMPUTING LABORATORY
De-novo sequencing
Produce and analyze large amounts of genomic sequence data from various origins (human, plants, bacteria…)
Develop bioinformatics tools for genome sequence analysis, annotation and exploration
Exploration of prokaryotic biological and biochemical diversity, for chemical and environmental applications

Sequencing multiples individuals from the same specie
Whole genome association studies, pan-genomic expression profiling, epigenetic studies, exome and whole genome sequencing
Research on the genetic of human diseases through internal and collaborative research programs
Searching for interaction between gene and environment
Precision / personalized medicine

Service for the academic community, through competitive call for projects.
Co-founded collaborative projects
In-house research projects : cross-fertilization between research and production
SEQUENCING INSTRUMENTS

5 HiSeq 2500
3 HiSeq 4000
1 HiSeqX5

- Sequencing for biodiversity projects
- De-novo sequencing
- Metagenomic
- Human exome
- Gene transcription (RNAseq)
- CHiPseq / epigenetic

- Whole genome sequencing
- Up to 9,000 whole genome / year

Third generation: single molecule, long reads, small footprint
A distributed infrastructure for genomic analysis and bioinformatic, publicly funded by the French government,
- 8 sequencing facilities, including the two national centers,
- 15 bioinformatics laboratories,
- A dedicated part of an HPC class system, ran by CEA HPC center (4,000 cores, 3 large memory systems (3 TB), 5 PB storage (HSM))

Objectives:
- sharing and leveraging expertise, providing high capacity resources for highly competitive projects,
- Technologies assessment (long reads, optical mapping…)
- methodology for sequencing and bioinformatics: assessment and development in relation to selected projects

9 work packages staffed with 45 temporary contracts for technology assessment and innovative developments – in collaboration with the French Institute for Bioinformatics (IFB)

Dedicated funding for large scale and high impact projects (direct costs), mainly on biodiversity and human genomic
Genomic is definitely in the Big Data arena


<table>
<thead>
<tr>
<th>Data Phase</th>
<th>Astronomy</th>
<th>Twitter</th>
<th>YouTube</th>
<th>Genomics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acquisition</td>
<td>25 zetta-bytes/year</td>
<td>0.5–15 billion tweets/year</td>
<td>500–900 million hours/year</td>
<td>1 zetta-bases/year</td>
</tr>
<tr>
<td>Storage</td>
<td>1 EB/year</td>
<td>1–17 PB/year</td>
<td>1–2 EB/year</td>
<td>2–40 EB/year</td>
</tr>
<tr>
<td>Analysis</td>
<td>In situ data reduction</td>
<td>Topic and sentiment mining</td>
<td>Limited requirements</td>
<td>Heterogeneous data and analysis</td>
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<tr>
<td>Analysis</td>
<td>Real-time processing</td>
<td>Metadata analysis</td>
<td></td>
<td>Variant calling, ~2 trillion central processing unit (CPU) hours</td>
</tr>
<tr>
<td>Analysis</td>
<td>Massive volumes</td>
<td></td>
<td></td>
<td>All-pairs genome alignments, ~10,000 trillion CPU hours</td>
</tr>
<tr>
<td>Distribution</td>
<td>Dedicated lines from antennae to server (600 TB/s)</td>
<td>Small units of distribution</td>
<td>Major component of modern user’s bandwidth (10 MB/s)</td>
<td>Many small (10 MB/s) and fewer massive (10 TB/s) data movement</td>
</tr>
</tbody>
</table>

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Data dynamic in Genomic: large raw data that expanse while processed (not true in HEP)

Summary: genomic = Big Data (3(+) V (Volume, Velocity, variability…)) + distributed computing

Need to efficiently feed hundreds if not thousands of CPU with living data
**Prerequisites for High Throughput Genomic:**
- Engineering, facilities: power, weight, cooling, space…
- Distributed computing, security, high performance IO

**Strategic partnership between the Genomic Institute and HPC teams,** in order to take into account genomics' specific needs:
- Medium and long term storage of living data,
- Data parallelism (easy for an HPC center), genome and metagenome assembly, classification, counting: large memory machine, long run time,
- Almost unpredictable execution time,
- Package availability, support for multiple concurrent versions,
- Groupware work mode

**Next move:** databases, data analytic
CEA operates several HPC centers, for Defense as well as for civilian applications.

- 4 systems in the 1-100th rank of Top500
- Expertise is shared among the systems
- Ready for exascale computing

Data centric model: civilian system shares the same storage.

**GL-TGCC**
- 7.5 PB disk
- Global (shared) Lustre servers

**ST-TGCC**
- Level 1: 1 PB disk
- Level 2: 30 PB tapes

Cobalt: 38,000 cores, 1.5 Pflops, 539 kW, 63th Top500

Curie, thin nodes: 78,000 cores, 1.6 Pflops,
«standard» Linux system, Slurm resources manager

«Modules» software management system, to deal with multiple versions, 
220+ software installed (genomic field), including many that depends on interpreters (Python, Perl, R…) whose versions may be incompatible

zyx

«Modules» also used for users directory selection (one user / multiple projects)

$ module load extenv/fg

$ module load dfldatadir/fgXXXX

$ module load samtools

$ module load vcf tools/0.1.12

loads FG extension, ie modules shown above)

(loads FG specific variables, for easier access to per-project data directory)

(loads default version of samtools)

(loads a specific version of samtools)
Main goal: to keep (large) files at only one place
- Web site (and authentication) located in users’ premise
- Read only access
- Technical details: reverse proxy
DAILY WORKLOAD

- Limit as much as possible data transfer: data are either stored locally or at the HPC premises, but not both.

- Accommodates production as well as research/exploration workflow. Though not “clinical-ready”

- Daily genotyping center production for WES and WGS run at the HPC premises,

- De-novo sequencing (assembly) for genomes and metagenome (including eukaryotic)
  - Example: Tara-Oceans projects (eukaryotic marine metagenomic and metatranscriptomic, 200 stations, 3 depth, 4 filter sizes), set up of a gene set of 180 millions entries, genomes and transcripts mapping (species abundance and functional activity).
OS based checkpoint and restart feature for application that lacks this and have long runtime

OS on demand, including Windows. With full data access.

Enlarge list of monitored and bookable resources (memory, IO...).
- Better restitution time guarantees.

From High Performance Computing to High Throughput Computing and Cloud features (on-demand, elasticity)
THANK YOU FOR YOUR ATTENTION. QUESTIONS?