Big data and HPC on-demand: Large-scale genome analysis on Helix Nebula – the Science Cloud

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ESA/ESRIN Frascati, 16 January 2013

EMBL

HELIX NEBULA
THESCIENCECLOUD

EMBL: European Molecular Biology Laboratory

- Intergovernmental Research Organization
- Supported by 20 Member States (+1 associated:)
- One of the world‘s foremost life science institutions
- EIROforum member
- 1500 staff
  >70 nationalities

The Five Branches of EMBL

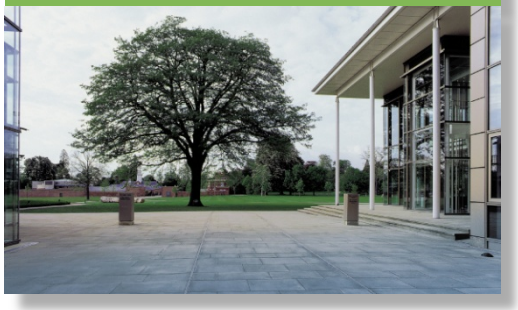
Heidelberg

Basic Molecular Biology Research
Main Lab / Headquarters

Hamburg

Structural Biology
DESY

Hinxton



European Bioinformatics Institute (EBI)
Sanger Centre

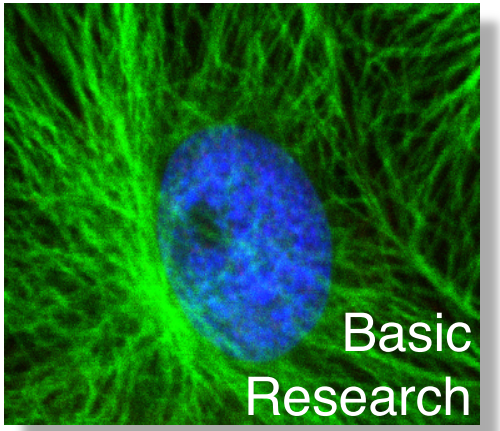
Grenoble

Structural Biology
ILL, ESRF, IBS, UVHCI

Monterotondo

Mousebiology
CNR, EMMA

EMBL's Missions



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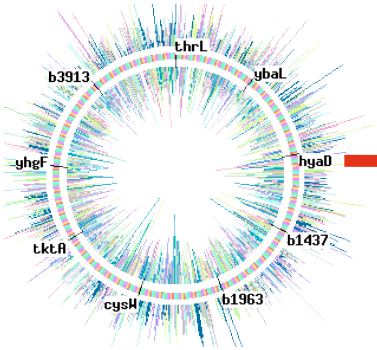
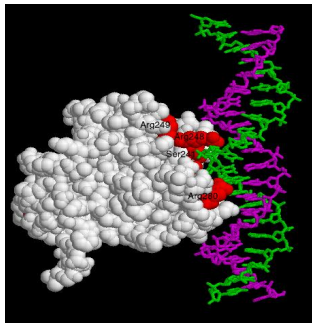
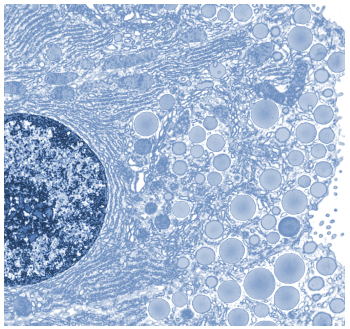
Systems Biology: From Molecules to Organisms



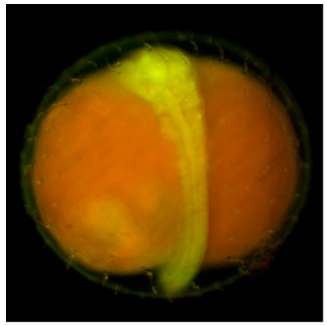
Genome



Protein/DNA

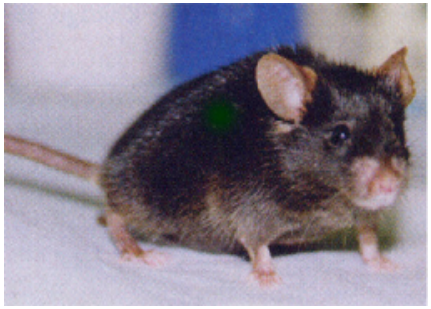


Cell



Embryo

Development



Organisms

Complexity

Aging

Disease

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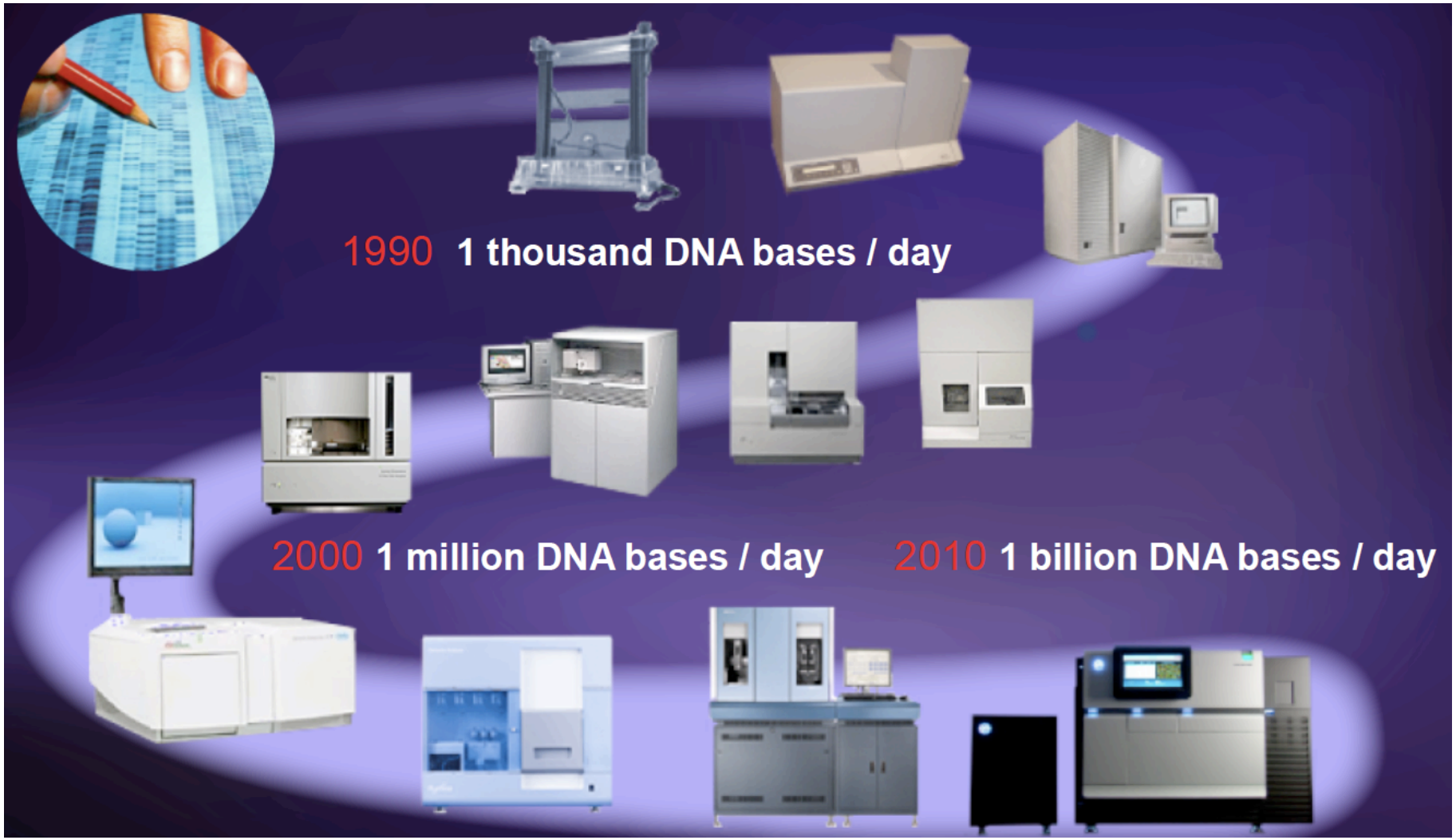
Next Generation Sequencing (NGS) Revolution



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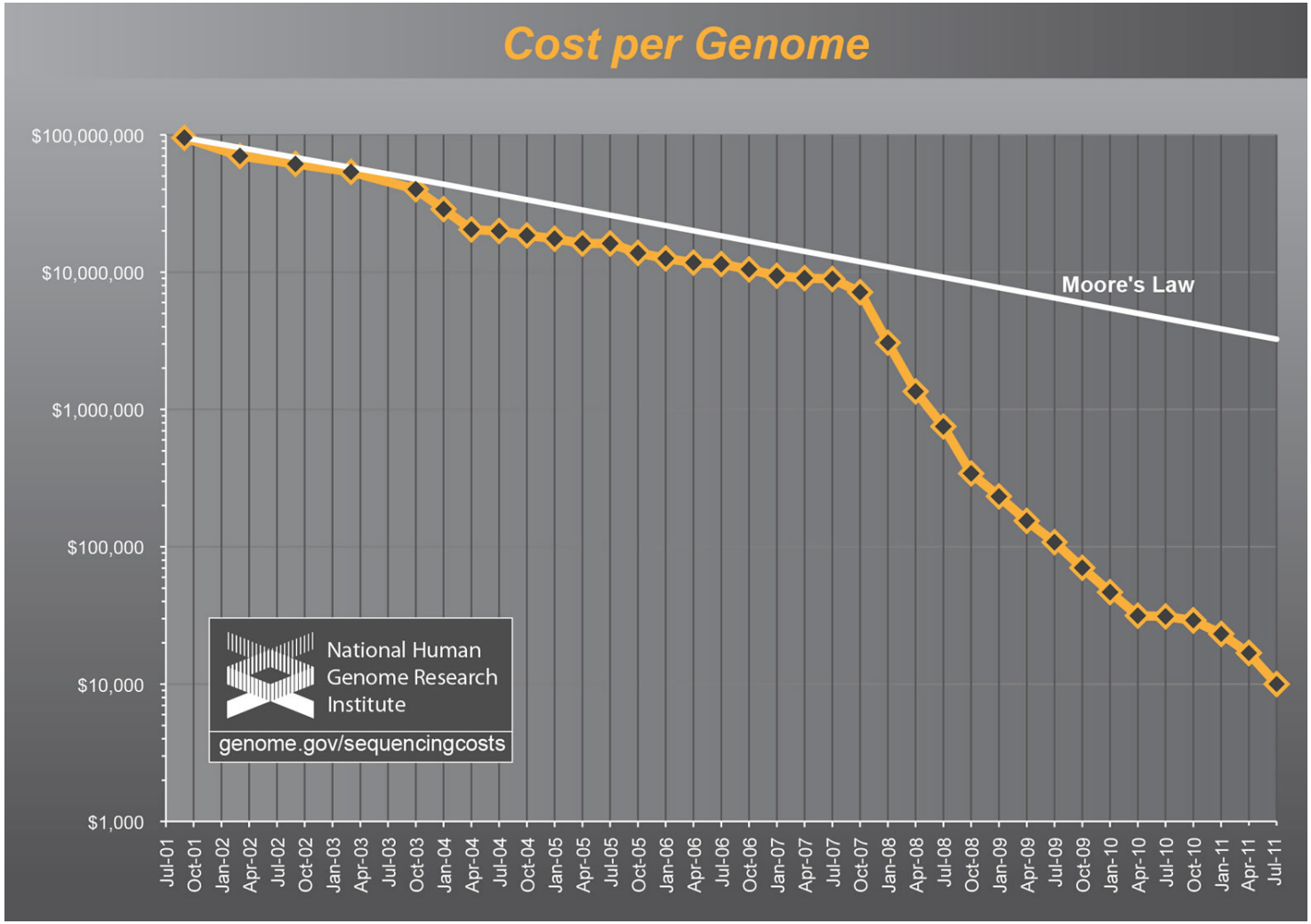
Cost of Sequencing Decreasing Rapidly



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Genomic Sequencing is Now an Affordable Solution

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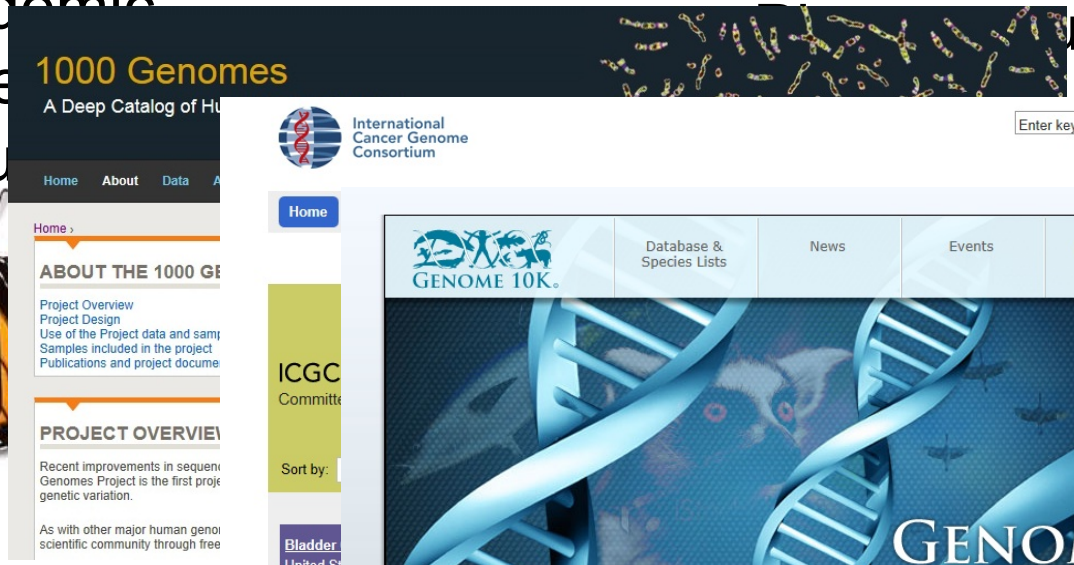

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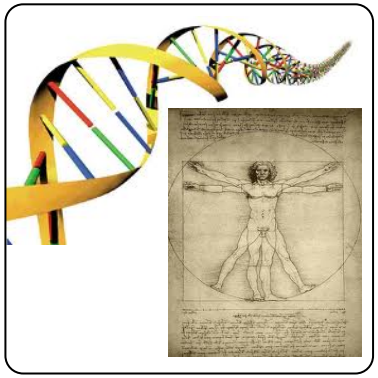
Genomic sequencing is
now an affordable solution

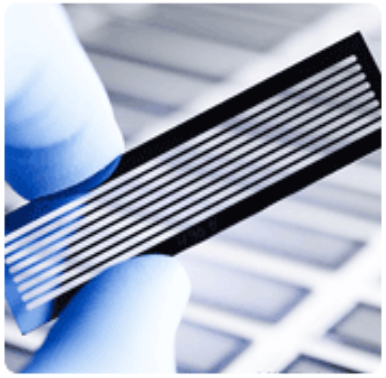
however ...

Read the Sequence to Study the Organism

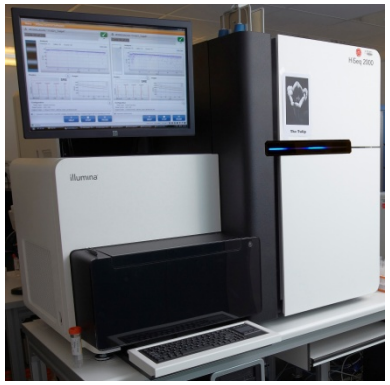
Extract DNA



Prepare



Sequence

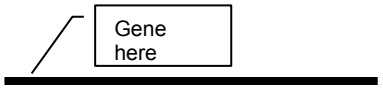


Lab

In Silico

Assemble

Annotate



Requires Computing Infrastructure & Expertise

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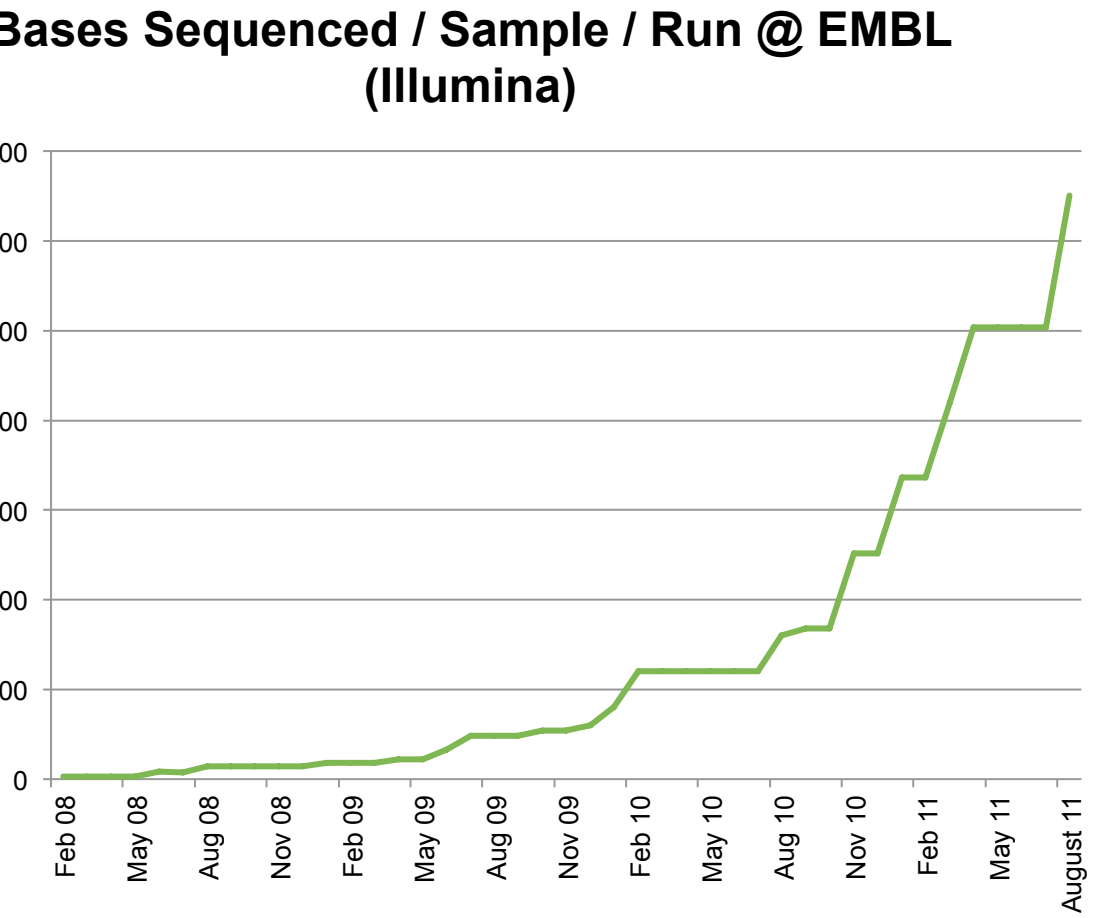
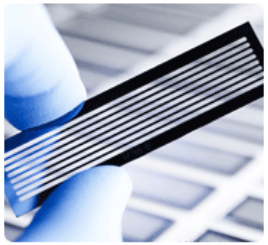
Problem - Technology Explosion with NGS





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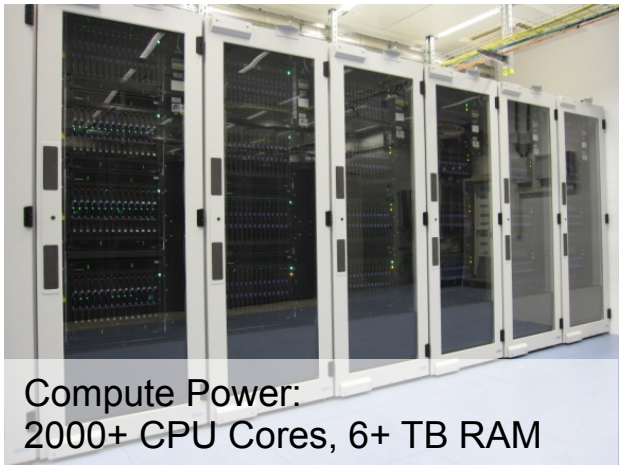
Sequence Production & IT Infrastructure at EMBL

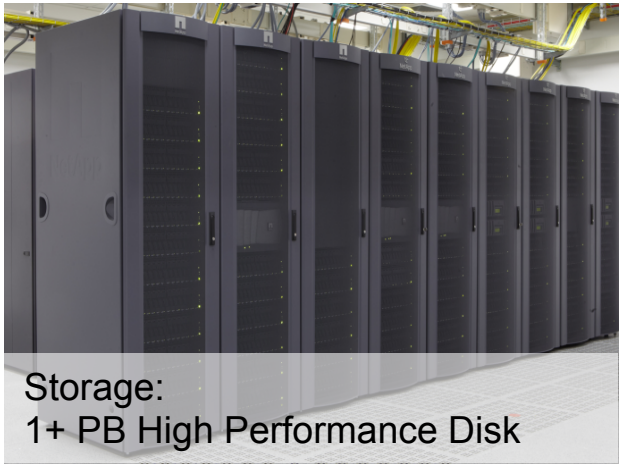
4 x Ilumina HiSeq2000

25+ TB data each week



1 x MySeq

1 x Ion Torrent



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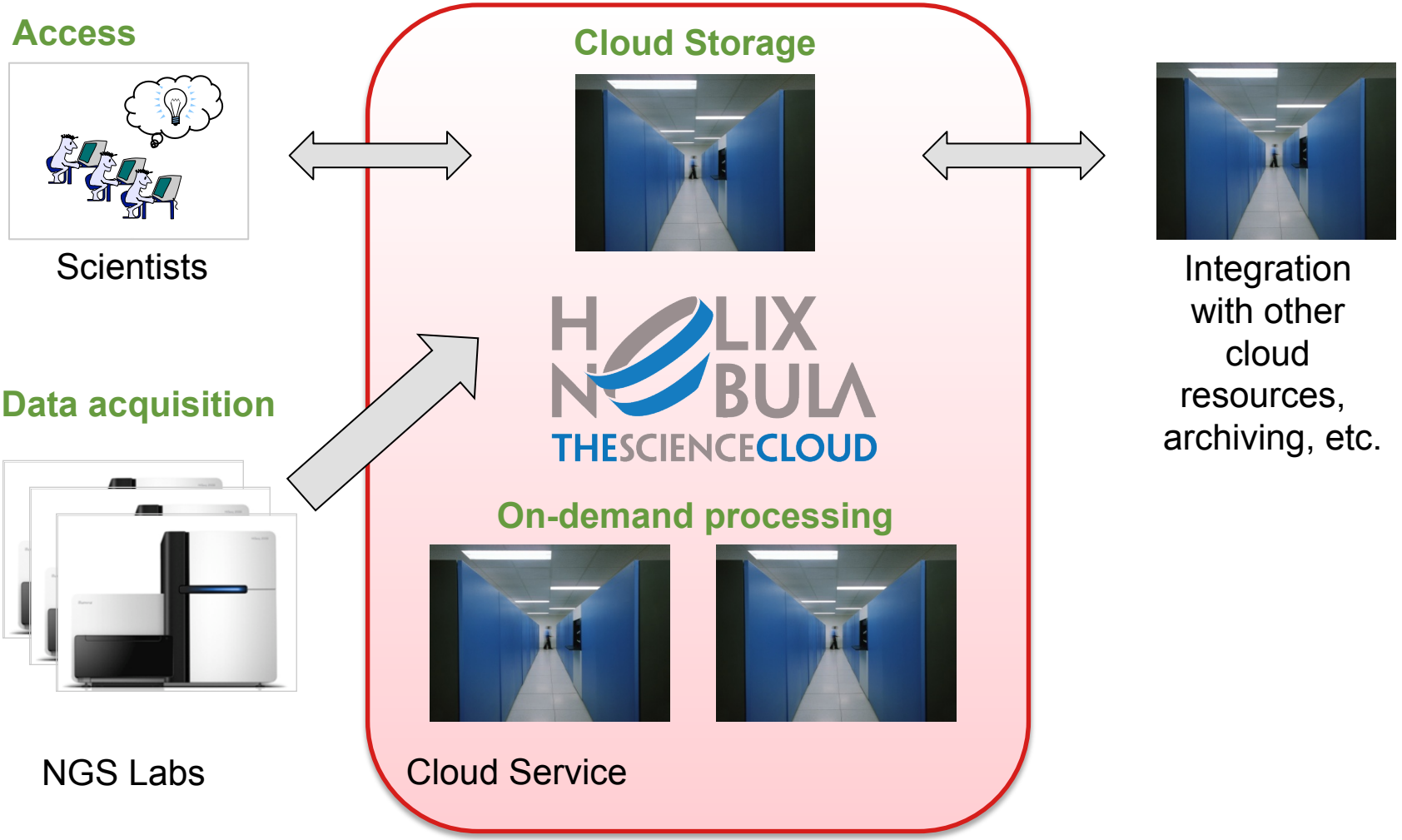
NGS - The Big Picture

- ~ 8.7 million species in the world (estimate)
- ~ 7 billion people
- Sequencers exist in both large centres & small research groups
- 200+ Ilumina HiSeq sequencers in Europe alone
  - capacity to sequence 1600 human genomes / month
- Largest centre: Beijing Genomics Institute (BGI)
  - ~140 HiSeq
- ~1500 Hiseq devices worldwide today
  - 3-6 PB / day
  - 1.1 – 2.2 ExaBbytes / year

EMBL Flagship: Large-scale Genome Analysis



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Proof of Concept

- Multiple Cloud providers
  - ATOS / Sixsq
  - CloudSigma
  - T-Systems
- Each tested steps with increasing complexity
- Major software components to test

Assembly pipeline	SGA by Simpson, JT & Durbin, R http://genome.cshlp.org/content/22/3/549.long
Annotation pipeline	Ensemble
Shared File system	e.g. glusterFS
StarCluster	http://star.mit.edu/cluster/

StarCluster & Sun Grid Engine
Dynamic cluster provisioning

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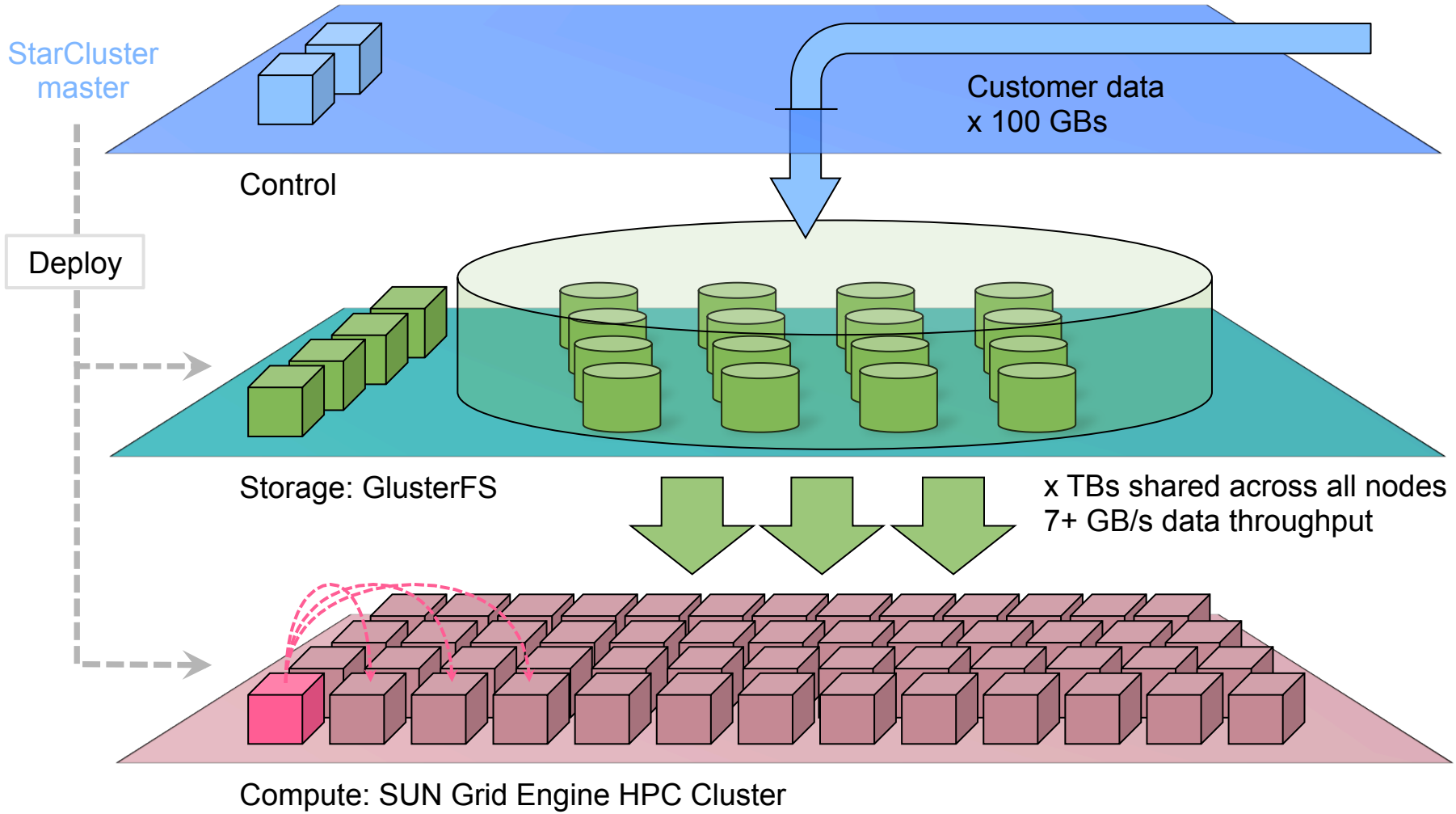
- StarCluster – Dealing with the Fluctuating Workload
  - Manages provisioning of images and setting up of cluster
  - Requires sets of EC2 APIs to work
  - It monitors the number of jobs in the queue and launches more instances
  - Terminates them when no longer required

- Sun Grid Engine
  - Single image running in two modes – master/worker
  - Post-launch configuration

EMBL Dynamic Cloud Architecture



Sun Grid Engine cluster troughput

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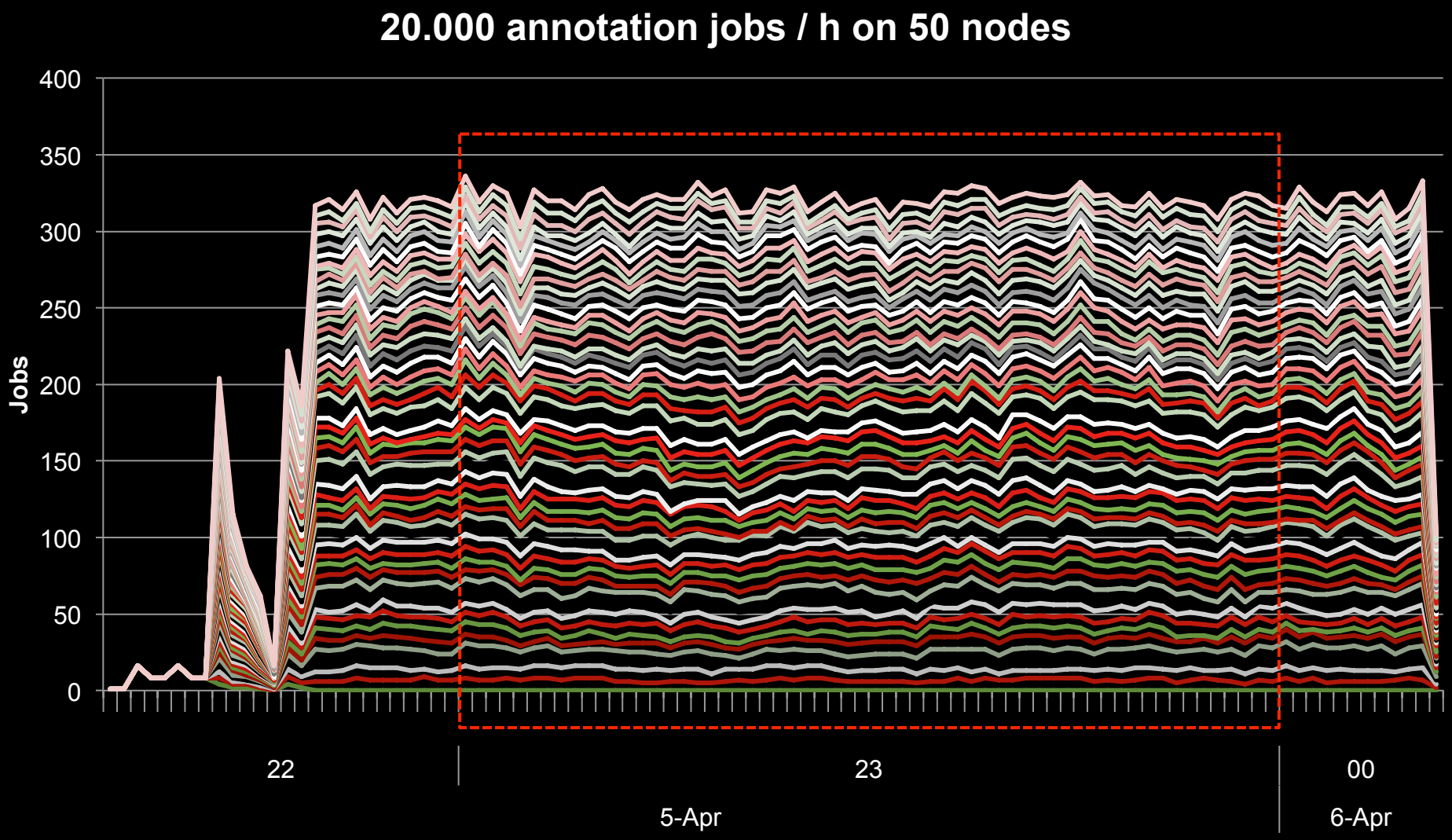

GlusterFS throughput

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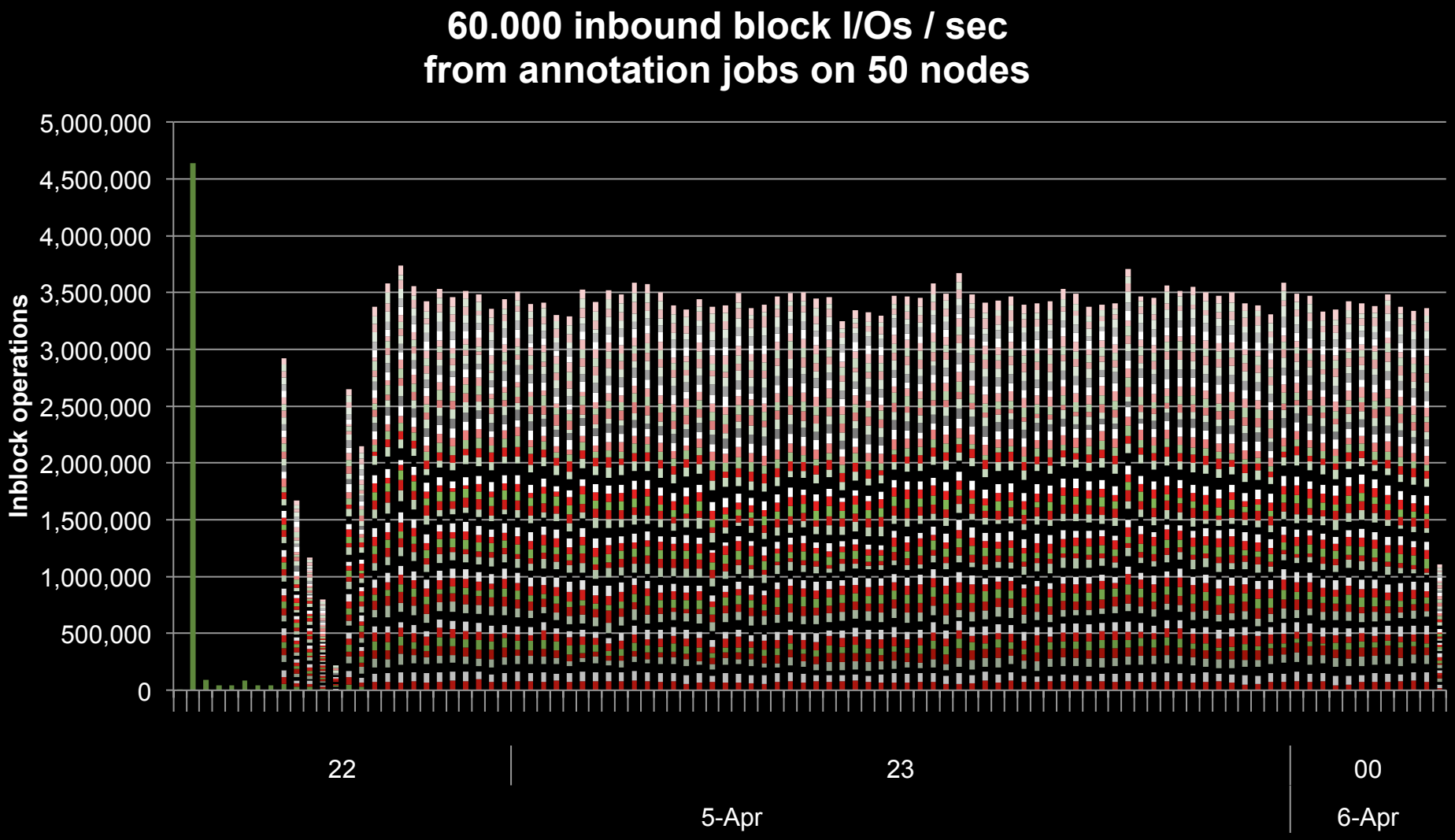
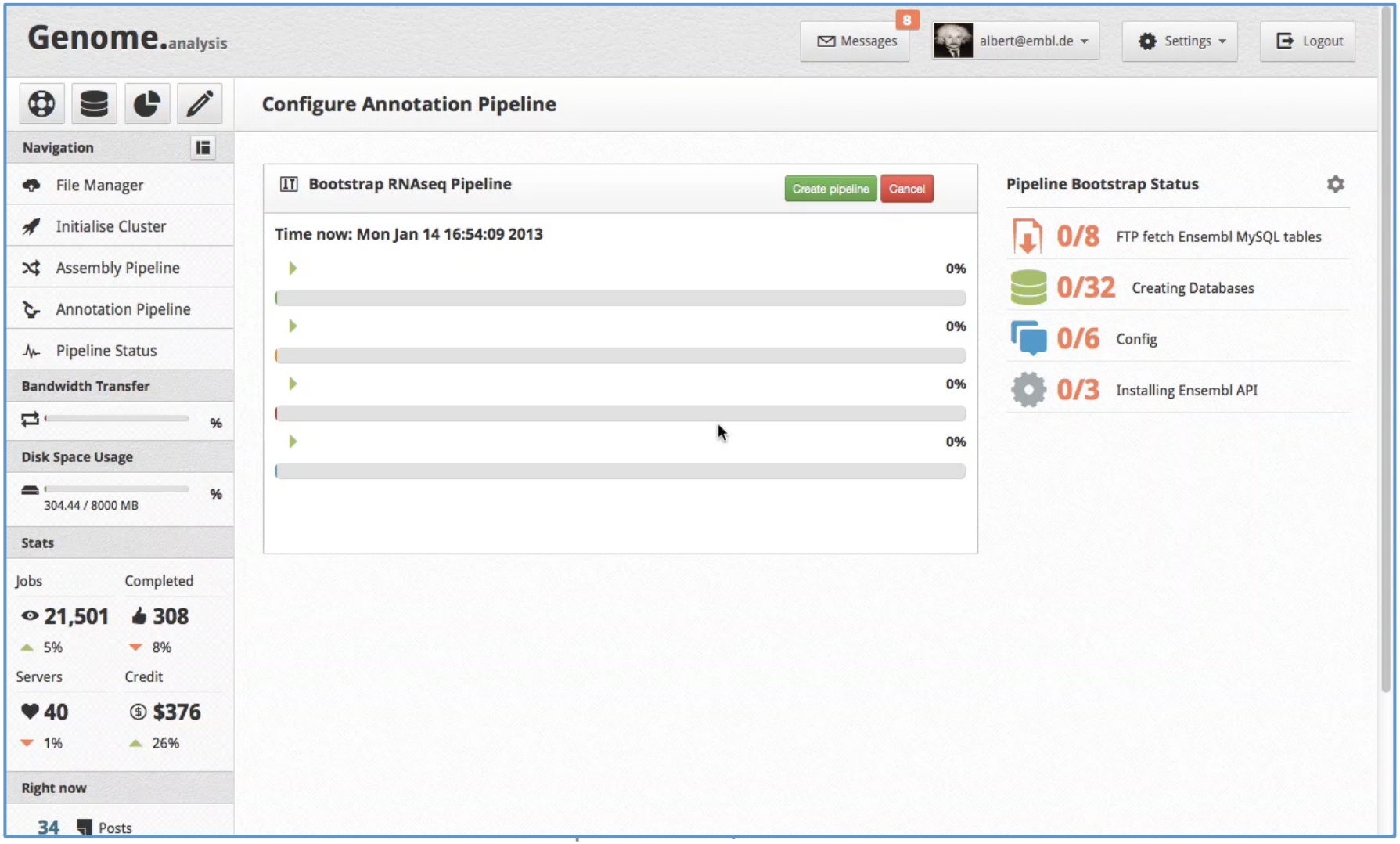


PoC results

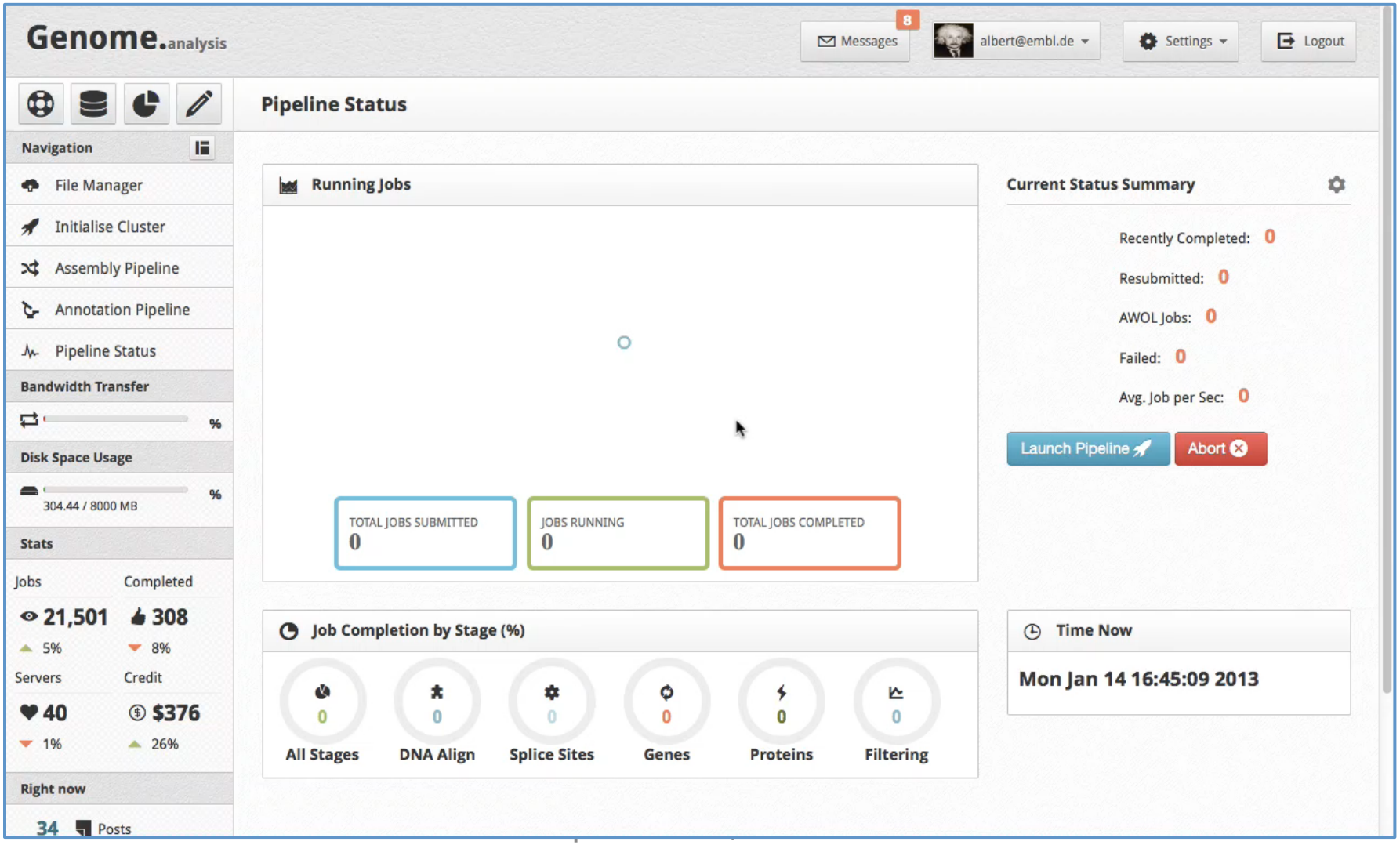
Successful tests of all vendors deployed so far

- StarCluster API integration
- auto-provision 50-node cluster setups
- real world large genome sequencing data
- 100,000s of jobs
- mix of quick parallel jobs and long running serial jobs
- glusterFS stability under high I/O levels
- Initial hurdles (e.g. image deployment, StarCluster integration, network setup) solved

User Interface Genome Analysis



User Interface Genome Analysis



Next steps

- Integration of EMBL flagship with first implementations of the Helix Nebula Blue Box
- Extensive testing of this federated cloud
- Feed back results to Helix Nebula requirements management
- Continue work on the UI
- Prepare for putting EMBL genome analysis pipeline into production in 2013

Helix Nebula PoC Acknowledgements

EMBL

Michael Wahlers
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Stephen Keenan
Paul Flicek

Atos

CloudSigma

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