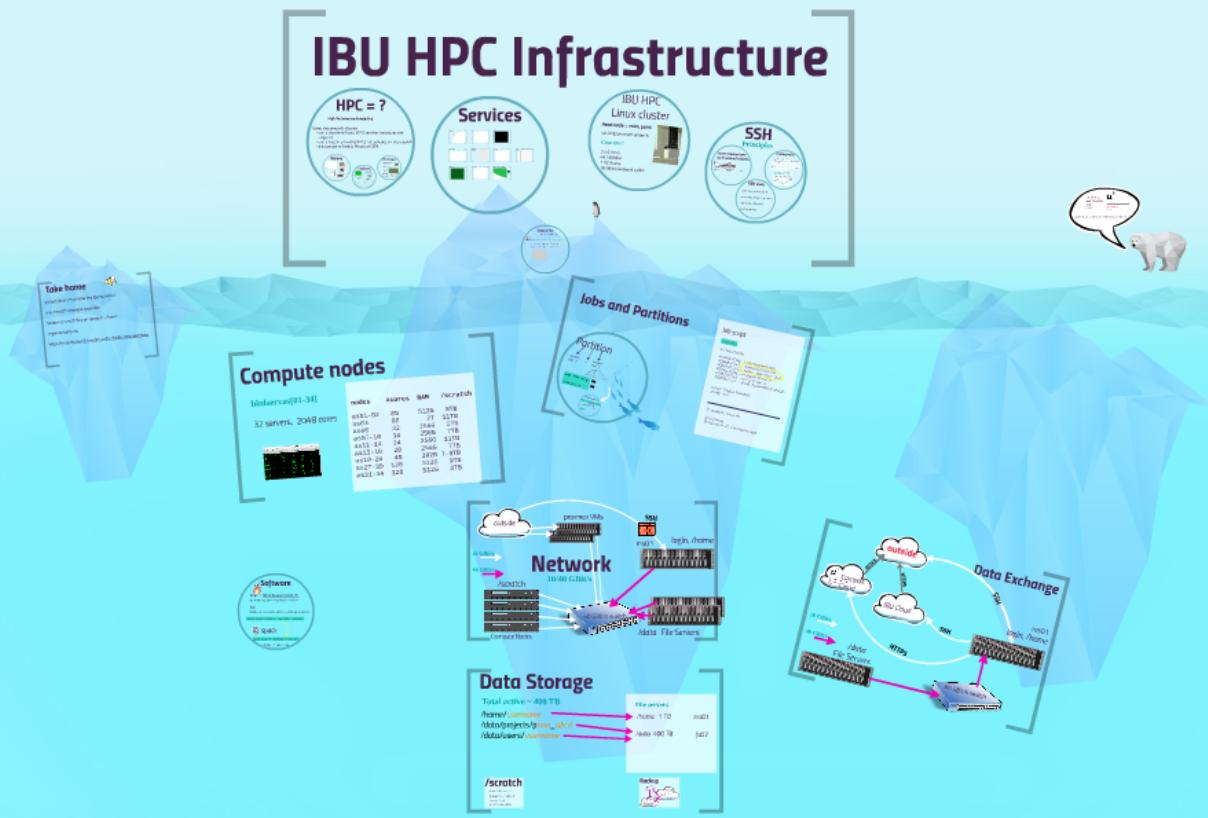


Interfaculty Bioinformatics Unit

Pierre Berthier, University of Bern, 26.10.2020



Interfaculty Bioinformatics Unit

Pierre Berthier, University of Bern, 26.10.2020

Interfaculty
Bioinformatics
Unit
(IBU)

u^b

b

**UNIVERSITÄT
BERN**

pierre.berthier@bioinformatics.unibe.ch



IBU HPC Infrastructure

HPC = ?

High Performance Computing

Using large amounts of power

- over a short time (hours) (HPC): weather forecast, genetic diagnostic
- over a long time (months) (HPC): Astrophysics, climate research
- grid computing: Particle Physics at CERN



Services

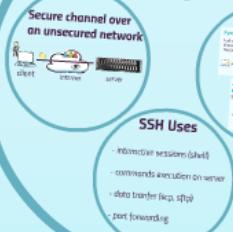


IBU HPC Linux cluster

Head node = entry point
ssh binfservms01.unibe.ch
Cent OS 7
2 x 6 cores
64 GB RAM
1 TB /home
10 GBit/s Network uplink



SSH Principles



Job script
test.sh
#!/bin/bash
#SBATCH

Jobs and Partitions

Partition



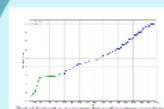
HPC = ?

High Performance Computing

Using large amounts of power

- over a short time (hours) (HPC): weather forecast, genetic diagnostic
- over a long time (months) (HTC): Astrophysics, climate research
- grid computing: Particle Physics at CERN

History



Features



Challenges

Electrical Power

Piz Daint: 3 MW
IBU: 15 kW
My Laptop: 60 W
City of Bern: 114 MW



Cooling

IBU Cluster: 1 PB Data
Uptime: 10 GB/s/s
(10-50 days to travel)
CDS cooling



Data flow

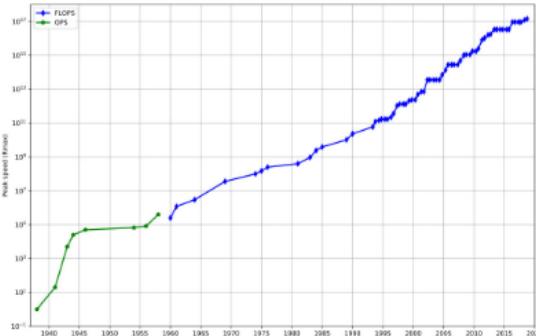
IBU Cluster: 1 PB Data
Uptime: 10 GB/s/s
(10-50 days to travel)



Internal Network



History



Plot of highest supercomputer performance over time
(wikipedia)

Ubelix, 6300 CPUs



picture: M. Rolli

IBU Cluster, 1888 CPUs



My Laptop, 8 CPUs

IBM BlueGene/P, 2007
23 TFLOPS, 65'536 CPUs

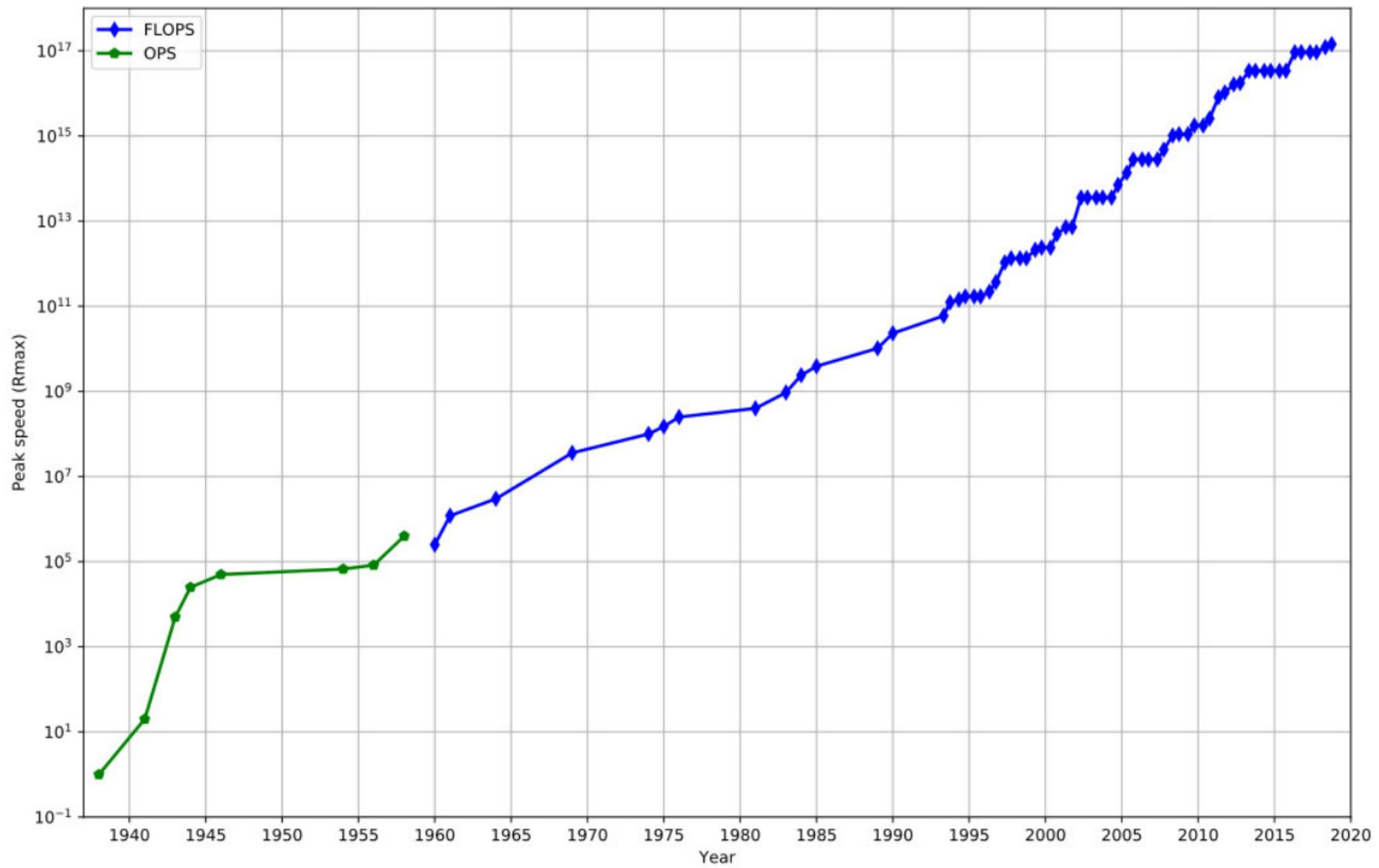


picture: wikipedia

Cray XC50, 2017, 27 PFLOPS
133'716 CPUs (Piz Daint, CSCS)



picture: wikipedia



Plot of highest supercomputer performance over time
(wikipedia)



picture: wikipedia

Cray-1, 1976, 160 MFLOPS

Smartphone, 2013: 1GFLOPS



picture: wikipedia

IBM BlueGene/P, 2007
23 TFLOPS, 65'536 CPUs

picture: wikipedia



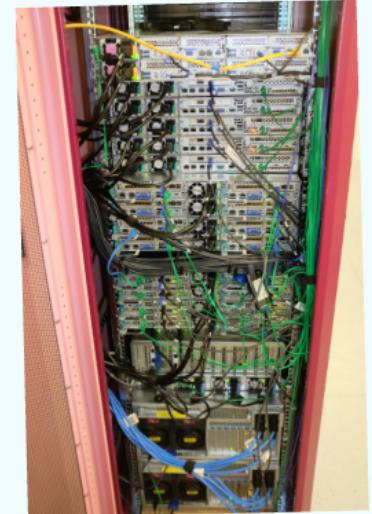
Cray XC50, 2017, 27 PFLOPS
133'716 CPUs (Piz Daint, CSCS)

Ubelix, 6300 CPUS



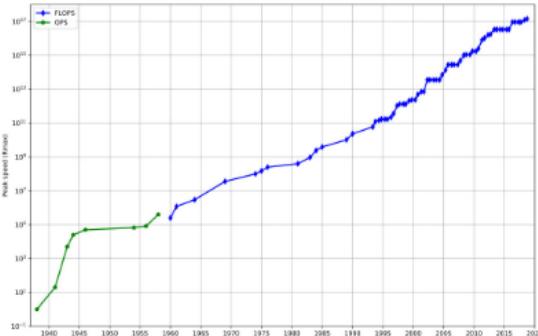
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IBU Cluster, 1888 CPUs



My Laptop, 8 CPUs

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Plot of highest supercomputer performance over time
(wikipedia)

Ubelix, 6300 CPUs



picture: M. Rolli

IBU Cluster, 1888 CPUs



My Laptop, 8 CPUs



picture: wikipedia

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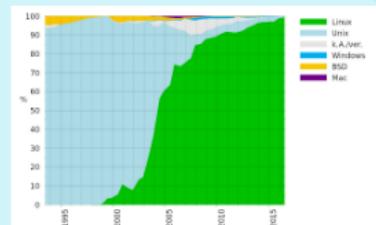


picture: wikipedia

Cray XC50, 2017, 27 PFLOPS
133'716 CPUs (Piz Daint, CSCS)

Features

Operating System

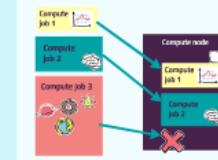


Operating systems used on top 500 supercomputers (wikipedia)

Queuing System

Concurrency on resources (CPUs, RAM) for users and jobs

Optimal usage of resources



Storage

Large capacities

1 Hard Disk: 16 TB

Piz Daint: 8'000 TB

Ubelix: 3'000 TB

IBU: 1'000 TB

High number of files

typically: 100's of millions of files

Network

Nodes Interconnect

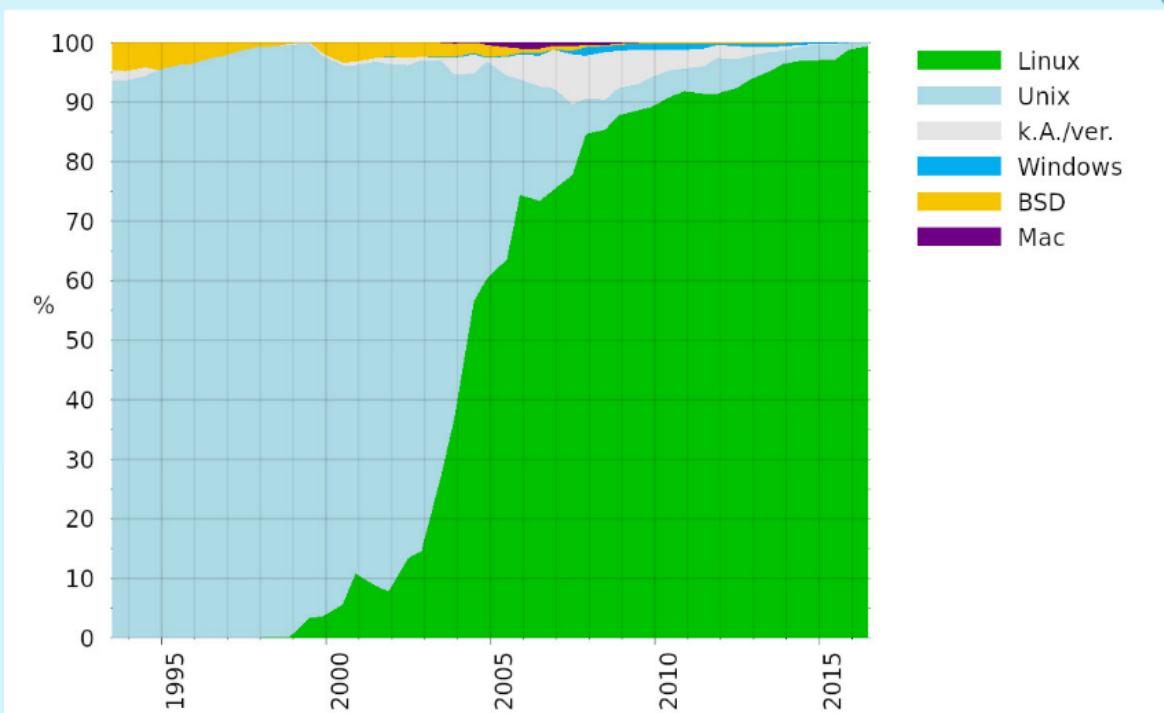
Typical: 10-56 Gbit/s

Network type: TCP/IP or infiniband

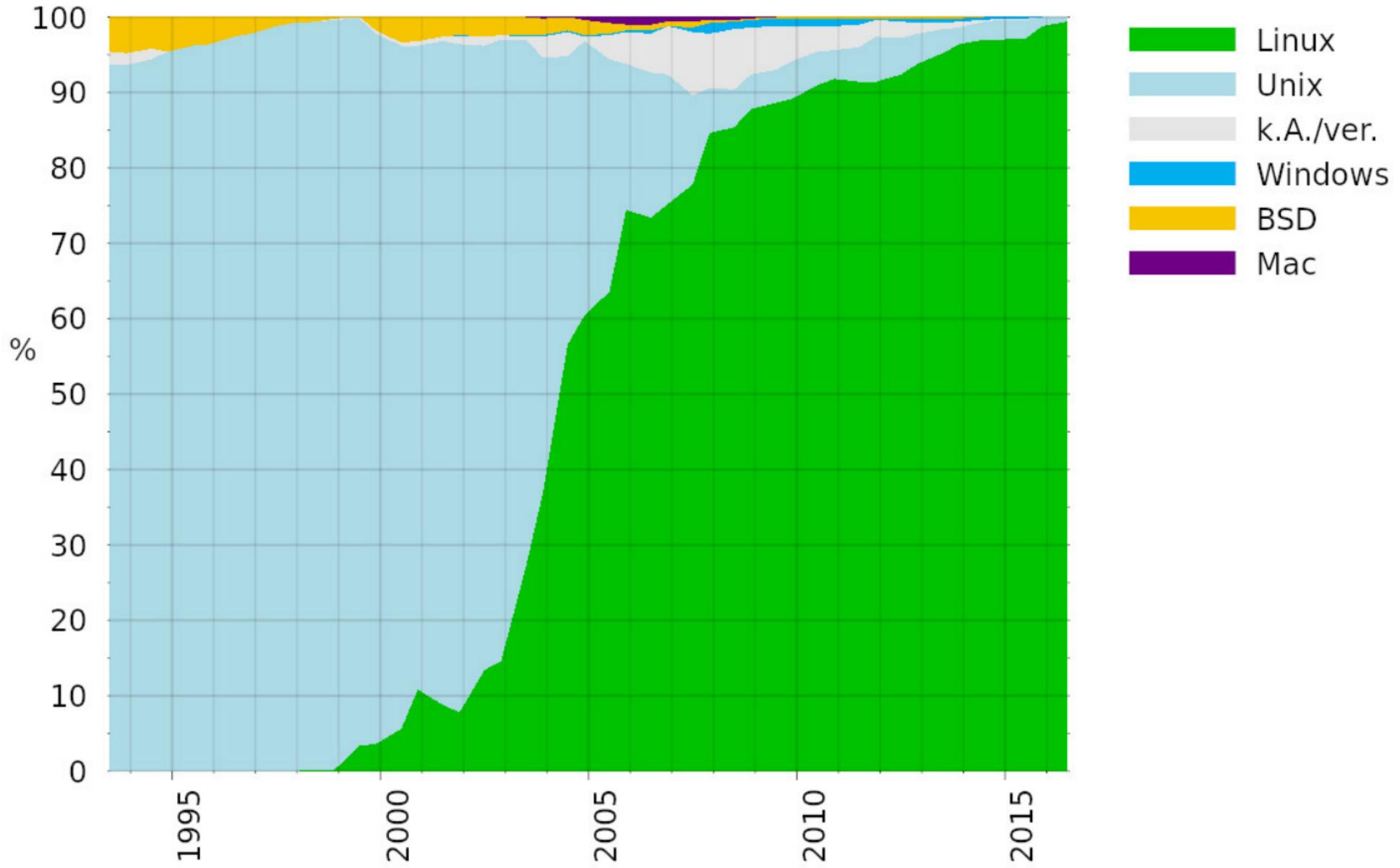
Outbound connection

Typical: 10 GBit/s

Operating System



Operating systems used on top 500 supercomputers (wikipedia)



Operating systems used on top 500
supercomputers (wikipedia)

Storage

Large capacities

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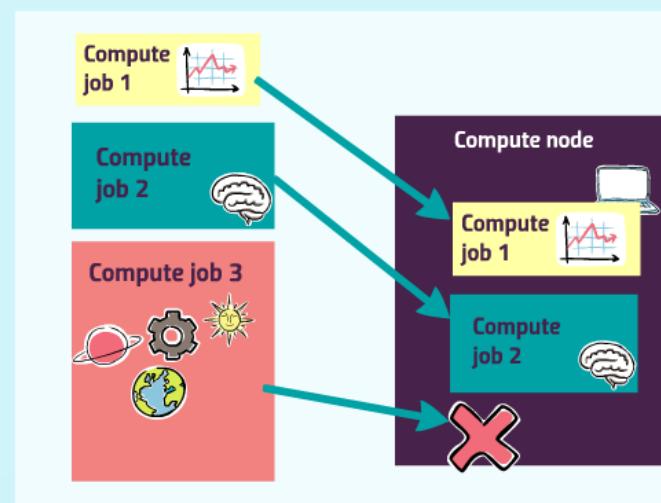
Outbound connection

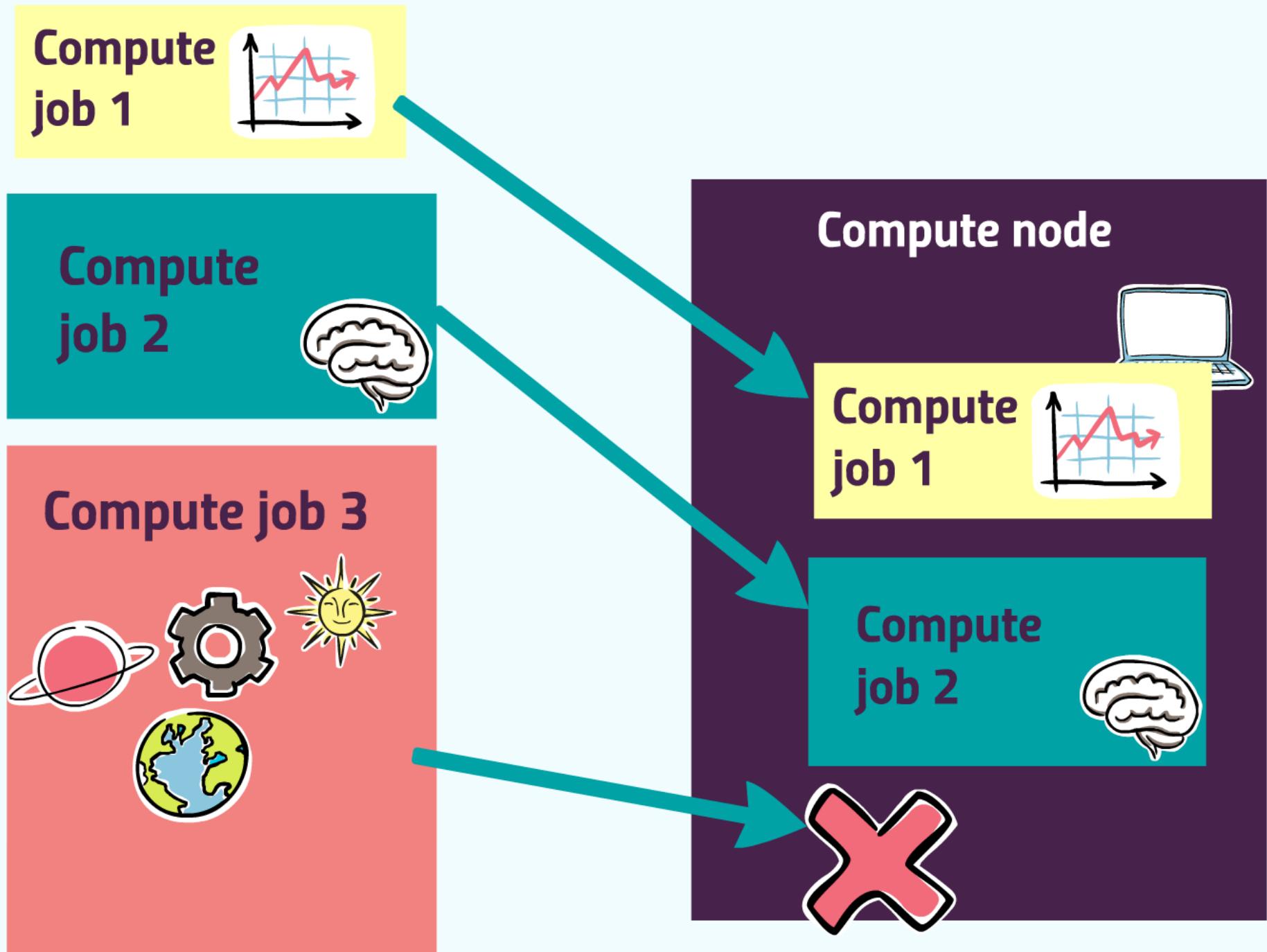
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Challenges

Electrical Power

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City of Bern: 114 MW



Cooling



CSCS cooling

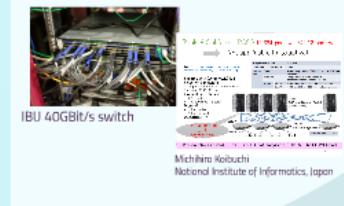
Data flow

IBU Cluster: 1 PB Data

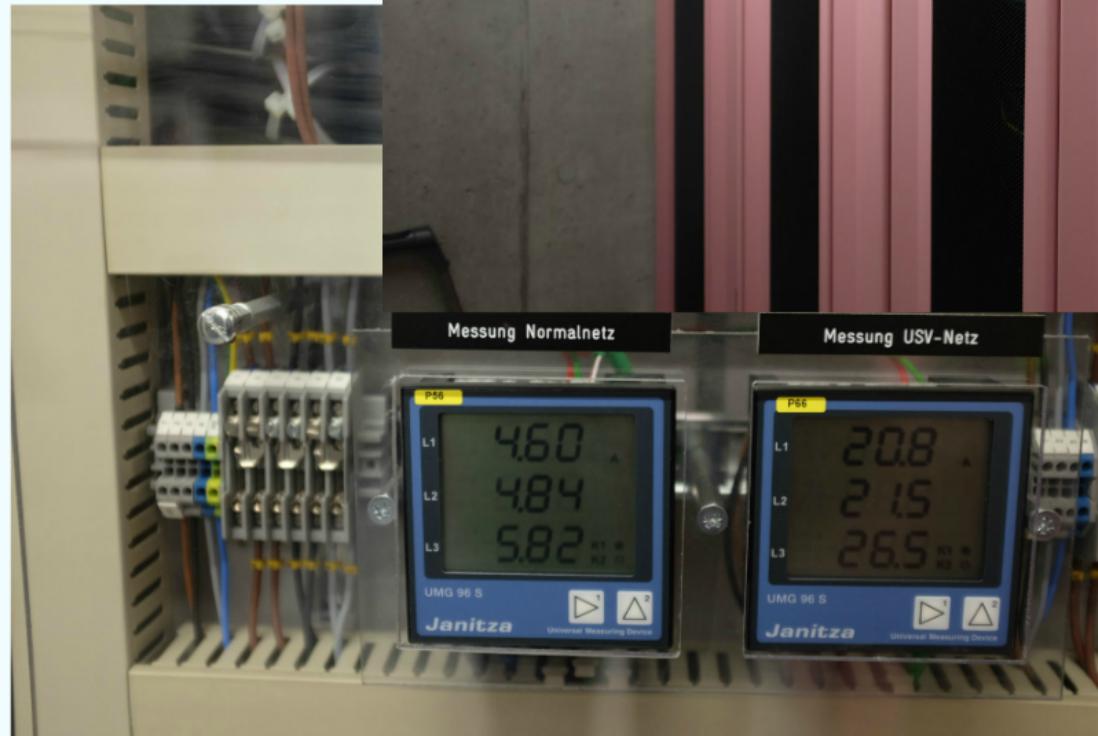
Uplink: 10 GBit/s

(10-50 days to transfer)

Internal Network



IBU HPC



Challenges

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Cooling



CSCS cooling

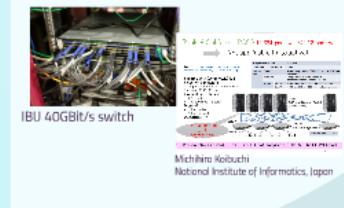
Data flow

IBU Cluster: 1 PB Data

Uplink: 10 GBit/s

(10-50 days to transfer)

Internal Network



Internal Network



IBU 40Gbit/s switch

Rank. 9 Oakforest-PACS: 12 384-port sw + 342 12-port sw

→ Not applicable for graphgolf

Ref [1] <https://www.ccs.tsukuba.ac.jp/wp-content/uploads/sites/14/2016/05/boku.pdf>

Fat-tree with (completely) full-bisection bandwidth

1 compute node == Intel® Xeon Phi™ Processor 7250 (68 cores)

of nodes/switches?

- 8208 nodes
- 362 switches (48 port)

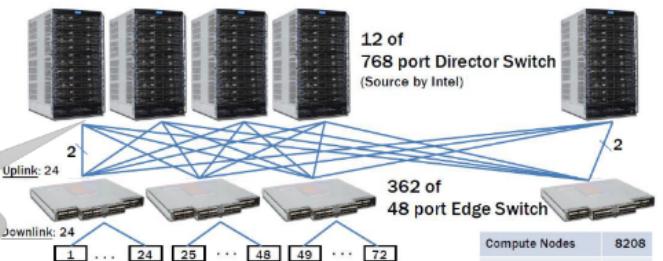
Degree? 48

- 24 for nodes
- 24 for network

Diameter: 2 or 4

2 cables per link
(Link Aggregation)

Total peak performance	25 PFLOPS
Total number of compute nodes	8,208
Compute node	Product
	Fujitsu Next-generation PRIMERGY server for HPC (under development)
Processor	Next-generation of Intel® Xeon Phi™ (Code name: Knights Landing), >60 cores
Memory	High BW 16 GB, >400 GB/sec (MCDRAM, effective rate) Low BW 96 GB, 115.2 GB/sec (DDR4-2400 x 6ch. peak rate)



→ Kohta Nakashima(FujitsuLab.), CSA Keynote (15:15–16:00, 29 Nov)

Michihiro Koibuchi
National Institute of Informatics, Japan

Rank. 9 Oakforest-PACS: 12 384-port sw + 342 12-port sw



Not applicable for graphgolf

Ref [1] <https://www.ccs.tsukuba.ac.jp/wp-content/uploads/sites/14/2016/05/boku.pdf>

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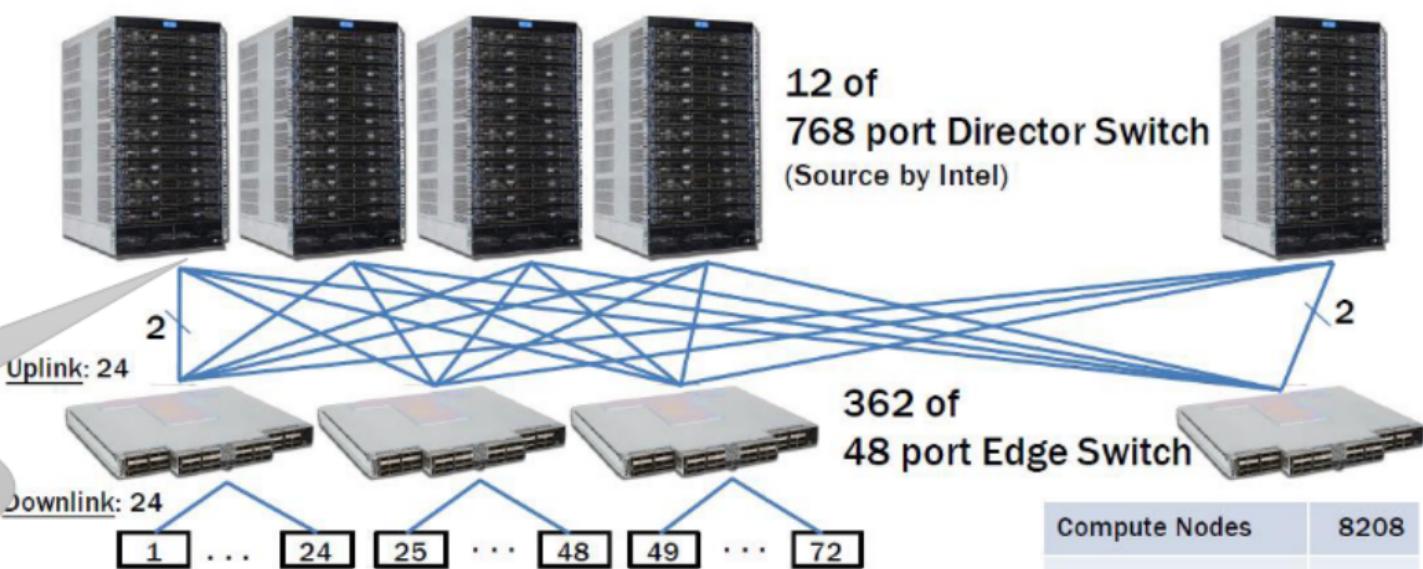
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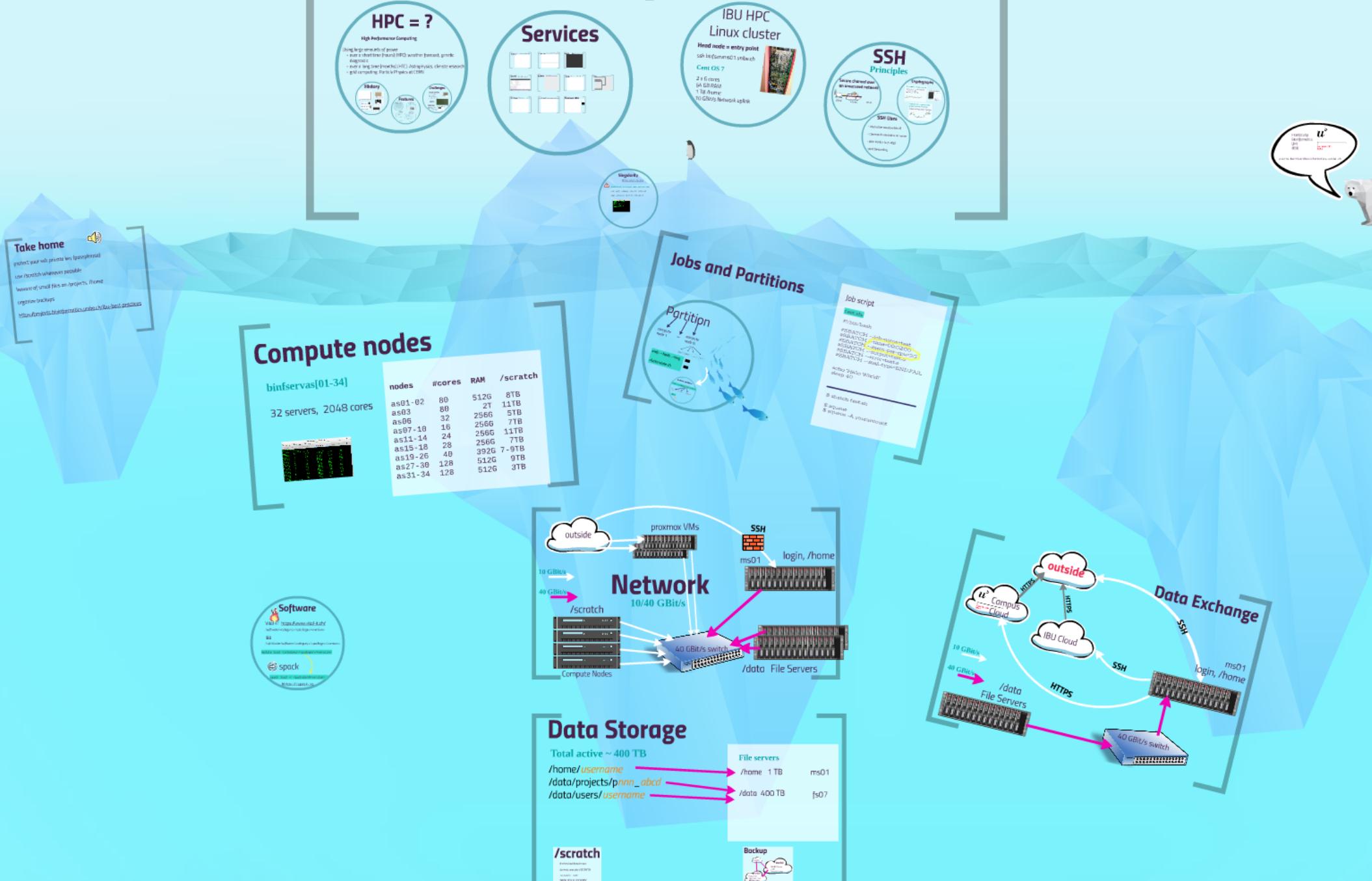
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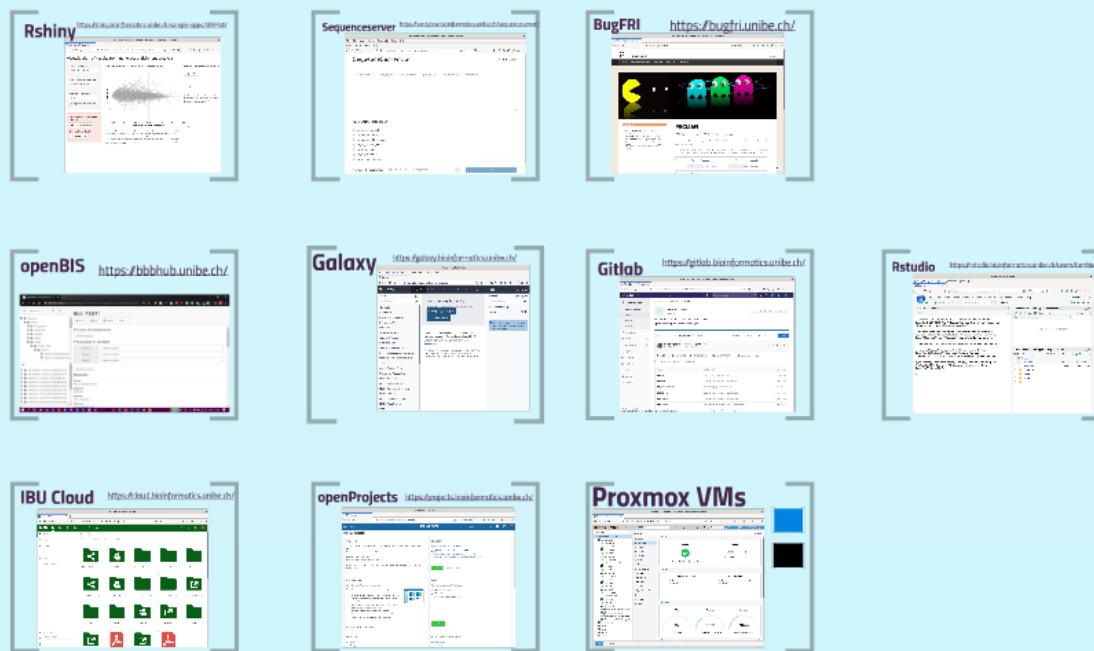


→ Kohta Nakashima(FujitsuLab.), CSA Keynote (15:15–16:00, 29 Nov)

IBU HPC Infrastructure

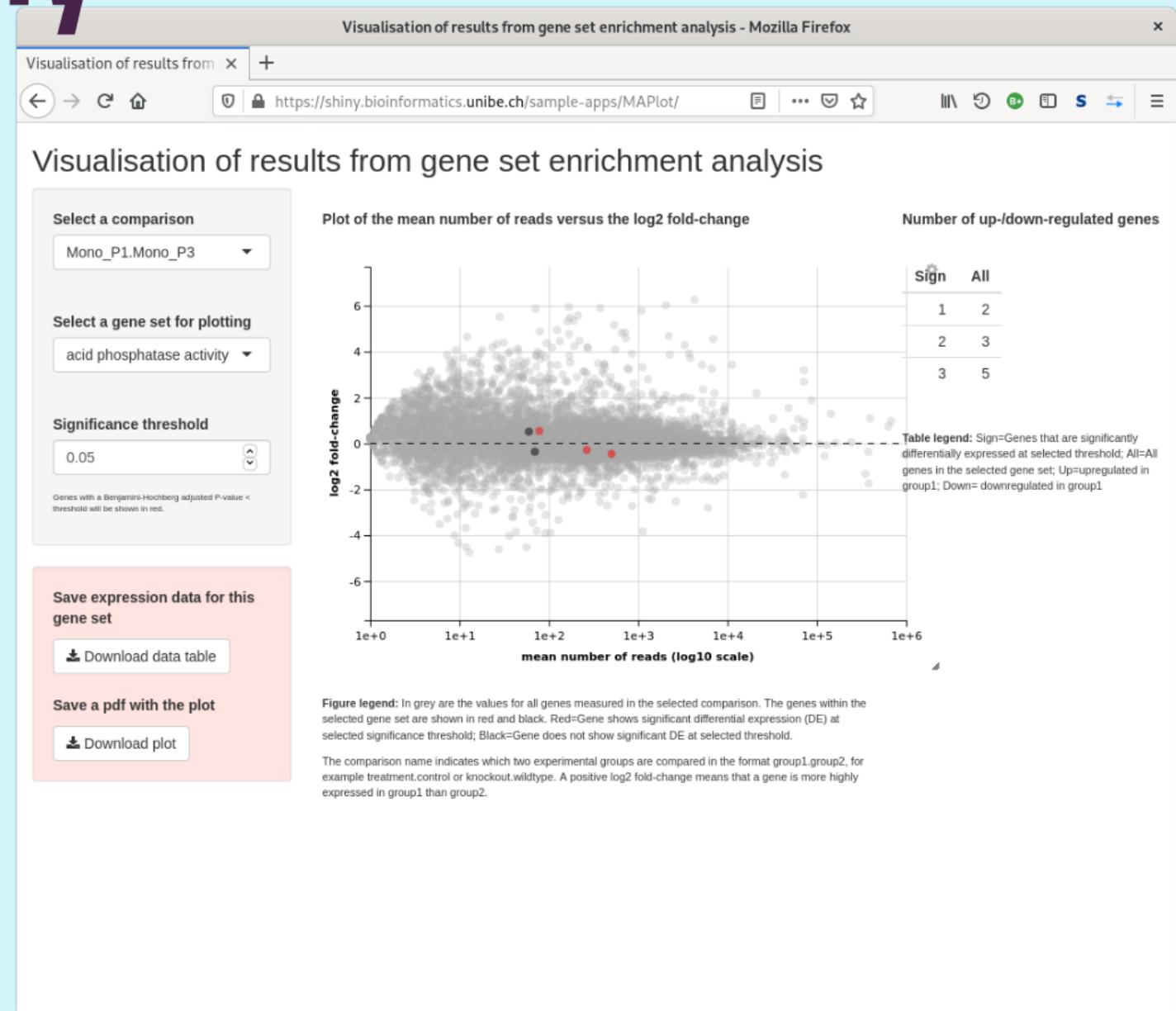


Services



Rshiny

<https://shiny.bioinformatics.unibe.ch/sample-apps/MAPlot/>



Sequenceserver

<https://xentobox.bioinformatics.unibe.ch/sequenceserver/>

The screenshot shows a Mozilla Firefox browser window with the title "SequenceServer: Custom BLAST Server - Mozilla Firefox". The address bar displays the URL <https://xentobox.bioinformatics.unibe.ch/sequenceserver/>. The main content area is titled "SequenceServer 1.0.11". A large text input field is present with the placeholder text "Paste query sequence(s) or drag file containing query sequence(s) in FASTA format here ...". Below this, a section titled "Nucleotide databases" lists several database options, each preceded by a checkbox:

- idm_dna_assembly.v1
- idm_rna_assembly_BE.v1
- idm_rna_assembly_Cannon.v1
- ssf_rna_assembly_BE.v1
- xnt_dna_assembly.v1
- xnt_dna_assembly.v2
- xnt_rna_assembly_all.v1

At the bottom, there is an "Advanced Parameters:" input field containing the text "eg: -eval 1.0e-5 -num_alignments 100", a help icon (?), and a blue "BLAST" button.

PACMAN: PACbio Methylation ANalyzer - Mozilla Firefox

PACMAN: PACbio Methylation ANalyzer https://bugfri.unibe.ch/

UNI FR UNIVERSITÉ DE FRIBOURG UNIVERSITÄT FREIBURG PACMAN

HOME MSC BIOINFORMATICS SEMINAR RESEARCH ABOUT US

Limitations

- The **contigs** smaller than 10'000bp are ignored.
- The **step** cannot be smaller than 500bp
- The **window** must be bigger than the step
- Maximum **4 motifs** are represented
- GFF** headers must correspond to **FASTA** headers

PACMAN

PACific biosciences Methylation ANalyzer

This web page allows a user to upload a bacterial full or draft genome, together with the motifs.gff file of a PacBio sequencing analysis.

The PACMAN web server will use Circos to generate a graphical view of the most important methylation motifs. The user can select among several possible views and filters. The output is a publication ready PDF or PNG.

Input FASTA (genome) ([example](#)) motifs.gff (Pacbio output) ([example](#))

No file selected. No file selected.

openBIS

<https://bbbhub.unibe.ch/>

The screenshot shows a web browser window for the openBIS platform at bbbhub.unibe.ch/openbis/webapp/eln-lims/?menuUniqueld=20181211162059617-92&v.... The main title is "Bbb: TEST1".

Left sidebar:

- Datasets
 - Others
 - Bruggmann
 - David Test
 - Default
 - Public
 - Yvesn
 - Project Test1
 - 20181211162058314-30
 - 20181211162058314-31

Top right actions:

- + New
- Edit
- Upload
- More ...

Process all comparisons:

Pick groups to compare:

Group by	-- select an option --
Group 1	-- select an option --
Group 2	-- select an option --

Start processing

Metadata:

Group:
IBU_University of Bern

Analysis:
RNA-Seq

Species:
Homo Sapiens

Platform:
Illumina HiSeq 2000

Bottom status bar:

96% 15:59 ENG

Galaxy

<https://galaxy.bioinformatics.unibe.ch/>

The screenshot shows the Galaxy web interface running on <https://galaxy.bioinformatics.unibe.ch/>. The browser title bar reads "Galaxy - Mozilla Firefox". The main content area displays a "Hello, Galaxy is running!" message with links to "Configuring Galaxy" and "Installing Tools". Below this, a paragraph describes Galaxy as an open platform for supporting data intensive research, developed by The Galaxy Team with contributions from many contributors. It also mentions the project's supporters: NHGRI, NSF, The Huck Institutes of the Life Sciences, The Institute for CyberScience at Penn State, and Johns Hopkins University. On the left, a sidebar titled "Tools" lists various tool categories: Get Data, Send Data, Collection Operations, Expression Tools, Lift-Over, Text Manipulation, Convert Formats, Filter and Sort, Join, Subtract and Group, Fetch Alignments/Sequences, Operate on Genomic Intervals, Statistics, Graph/Display Data, Phenotype Association, NGS: Mapping, NGS: RNA Analysis, NGS: QC and manipulation, NGS: SAMtools, NGS: Variant Analysis, NGS: Peak Calling, and Misc. On the right, a "History" panel shows an "Unnamed history" section which is currently empty.

Gitlab

<https://gitlab.bioinformatics.unibe.ch/>

The screenshot shows a Mozilla Firefox browser window displaying a GitLab project page. The URL in the address bar is <https://gitlab.bioinformatics.unibe.ch/berthier/spack-ibu-repos>. The page title is "Pierre Berthier / spack IBU repos · GitLab - Mozilla Firefox".

The left sidebar contains the following navigation links:

- S spack IBU repos
- Project overview
- Details (selected)
- Activity
- Releases
- Repository
- Issues (0)
- Merge Requests (0)
- CI / CD
- Operations
- Analytics
- Wiki
- Snippets
- Settings

The main content area shows the project details for "spack IBU repos" (Project ID: 11). It includes statistics: 12 Commits, 1 Branch, 0 Tags, and 625 KB Files. A description states "Spack Repository for IBU specific packages".

Below the stats, there is a commit history section with a single commit from Pierre Berthier: "new package py-mg-toolkit and dependencies" (authored 2 months ago, commit hash 5fe3f9dc). There are also buttons for "History", "Find file", "Web IDE", and "Clone".

Underneath the commit history, there are several dashed-line buttons for repository management: "README", "Add LICENSE", "Add CHANGELOG", "Add CONTRIBUTING", "Enable Auto DevOps", "Add Kubernetes cluster", and "Set up CI/CD".

A table lists the packages in the repository, showing their names, last commits, and last update times:

Name	Last commit	Last update
amos	corrections after flake8 tests	1 year ago
fastp	clean up comments and dependencies	2 months ago
genomethreader	new package genomethreader	2 months ago
libdatrie	clean up comments and dependencies	2 months ago
libdrmaa	clean up comments and dependencies	2 months ago
py-aiodns	new package py-mg-toolkit and dependencies	2 months ago
	new package py-mg-toolkit and dependencies	2 months ago

At the bottom of the page, the URL <https://gitlab.bioinformatics.unibe.ch/berthier/spack-ibu-repos> is repeated.

Rstudio

<https://rstudio.bioinformatics.unibe.ch/users/berthier/>

The screenshot shows the RStudio interface running in a Mozilla Firefox browser window. The title bar reads "RStudio - Mozilla Firefox".

Console pane:

```
R version 3.6.2 (2019-12-12) -- "Dark and Stormy Night"  
Copyright (C) 2019 The R Foundation for Statistical Computing  
Platform: x86_64-pc-linux-gnu (64-bit)  
  
R is free software and comes with ABSOLUTELY NO WARRANTY.  
You are welcome to redistribute it under certain conditions.  
Type 'license()' or 'licence()' for distribution details.  
  
Natural language support but running in an English locale  
  
R is a collaborative project with many contributors.  
Type 'contributors()' for more information and  
'citation()' on how to cite R or R packages in publications.  
  
Type 'demo()' for some demos, 'help()' for on-line help, or  
'help.start()' for an HTML browser interface to help.  
Type 'q()' to quit R.
```

Environment pane:

Global Environment

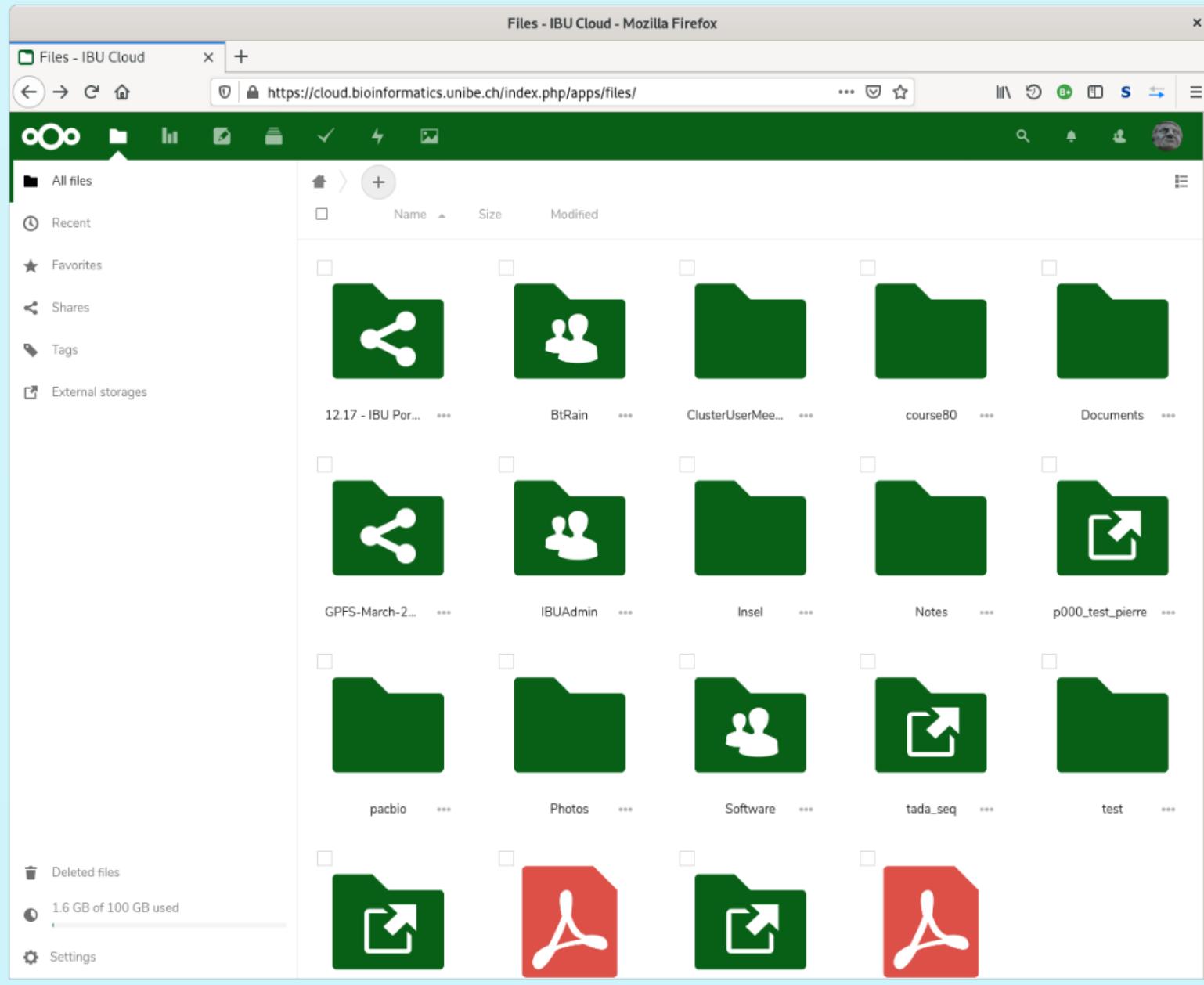
Environment is empty

Files pane:

Name	Size	Modified
.Rhistory	254 B	May 7, 2020,
CLUSTER		
p000		
p380		
R		

IBU Cloud

<https://cloud.bioinformatics.unibe.ch/>



openProjects

<https://projects.bioinformatics.unibe.ch/>

Proxmox VMs

binfsvpx01 - Proxmox Virtual Environment - Mozilla Firefox

binfsvpx01 - Proxmox

https://px01.binf.unibe.ch:8006/#v1:0:18:4::::5

You are logged in as 'root@pam' Documentation Create VM Create CT

PROXMOX Virtual Environment 5.4-13 Search

Server View

- Datacenter (IBU-MAIN)
 - binfsvpx01
 - 100 (app18)
 - 101 (des101)
 - 102 (app02)
 - 105 (app01)
 - 106 (app03)
 - 107 (des113)
 - 109 (binfsvapp13)
 - 111 (lic01)
 - 113 (app12)
 - 114 (app05)
 - 115 (binfldap01)
 - 117 (app17)
 - 119 (app09)
 - 120 (app10)
 - 121 (chef)
 - 123 (binfnfs02)
 - 125 (binfmonitor)
 - 129 (fs05)
 - 130 (app20)
 - 135 (app11)
 - binfsan01nfs (binfsvpx01)
 - local (binfsvpx01)
 - localdata-px01 (binfsvpx01)
 - localdata-px02 (binfsvpx01)
 - binfsvpx02
 - Apps
 - Test
 - allvms
 - critical

Tasks Cluster log

Datacenter

Health

Status

Nodes

Cluster: IBU-MAIN, Quorate: Yes

Online	2
Offline	0

Guests

Virtual Machines

Running	28
Stopped	3

LXC Container

Running	0
Stopped	0

Resources

CPU

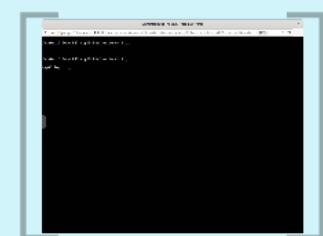
Memory

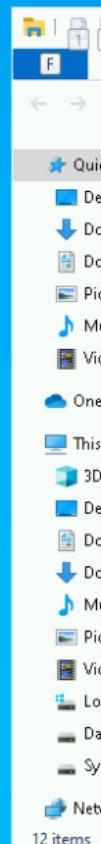
Storage

2% of 32 CPU(s)

30% 224.99 GiB of 755.64 GiB

39% 15.18 TiB of 39.18 TiB





Type here to search



File Explorer



FRA

7:50 AM
5/7/2020

File Explorer

F Home Share View

Quick access

Frequent folders (6)

- Desktop This PC
- Downloads This PC
- Documents This PC
- Pictures This PC
- Music This PC
- Videos This PC

Recent files (6)

- balloon
- netkvm
- qxlodod
- vioinput
- viostor
- vioscsi

CD Drive (D):\Balloon\w10\amd64

CD Drive (D):\NetKVM\w10\amd64

CD Drive (D):\qxlodod\w10\amd64

CD Drive (D):\vioinput\w10\amd64

CD Drive (D):\viostor\w10\amd64

CD Drive (D):\vioscsi\w10\amd64

12 items

QEMU (app08) - noVNC - Mozilla Firefox

x

https://px01.binf.unibe.ch:8006/?console=kvm&novnc=1&vmid=112&vmname=app08&node=binfservpx02&resize=off&cmd= 110% ... ☰ ☆

Ubuntu 18.04.4 LTS app08.binf.unibe.ch tty1

Ubuntu 18.04.4 LTS app08.binf.unibe.ch tty1

app08 login: _

IBU HPC Linux cluster

Head node = entry point

ssh binfservms01.unibe.ch

Cent OS 7

2 x 6 cores

64 GB RAM

1 TB /home

10 GBit/s Network uplink



SSH

Principles

**Secure channel over
an unsecured network**



SSH Uses

- interactive sessions (shell)
- commands execution on server
- data transfer (scp, sftp)
- port forwarding

Cryptography

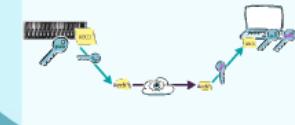
Symmetric cryptography

Goal: establish a secured channel
Shared secret
Key Exchange algorithm

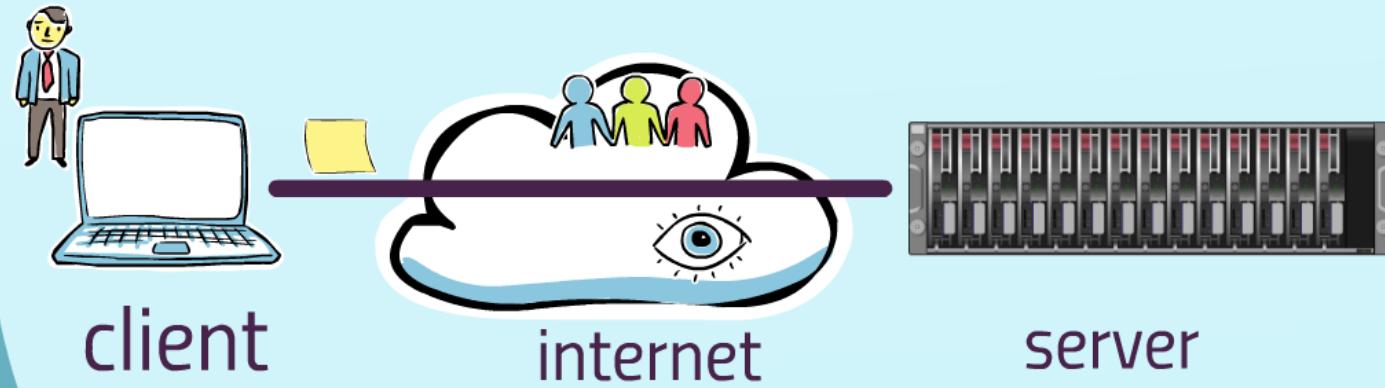


Asymmetric cryptography public/private keys pair

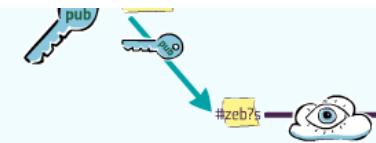
Server and User authentication



Secure channel over an unsecured network



SSH U



SSH Uses

- interactive sessions (shell)
- commands execution on server
- data transfer (scp, sftp)
- port forwarding

Cryptography

Symmetric cryptography

Goal: establish a secured channel

Shared secret 

Key Exchange algorithm



Key Exchange Algorithm

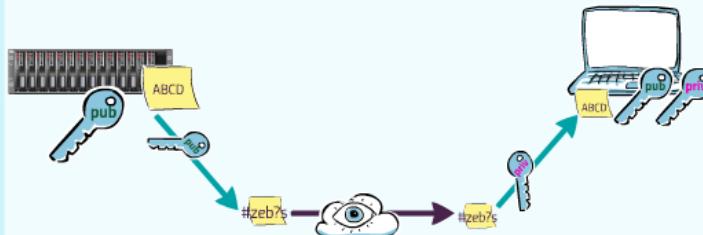
(Diffie-Hellman)



Source: wikipedia,
Original schema:
A.J. Han Vinck, University of
Duisburg-Essen

Asymmetric cryptography public/private keys pair

Server and User authentication



Uses

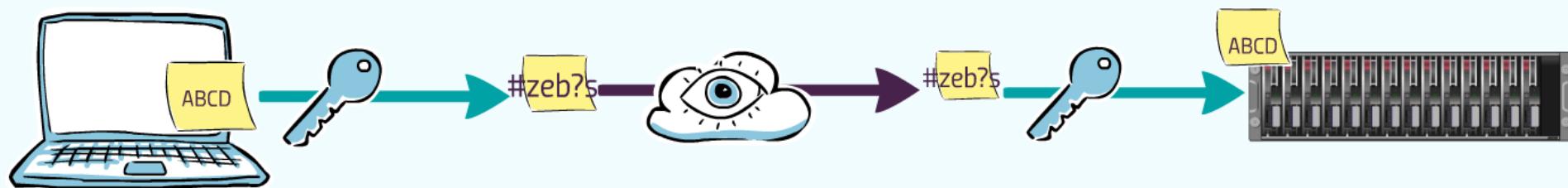
Symmetric cryptography

Goal: establish a secured channel

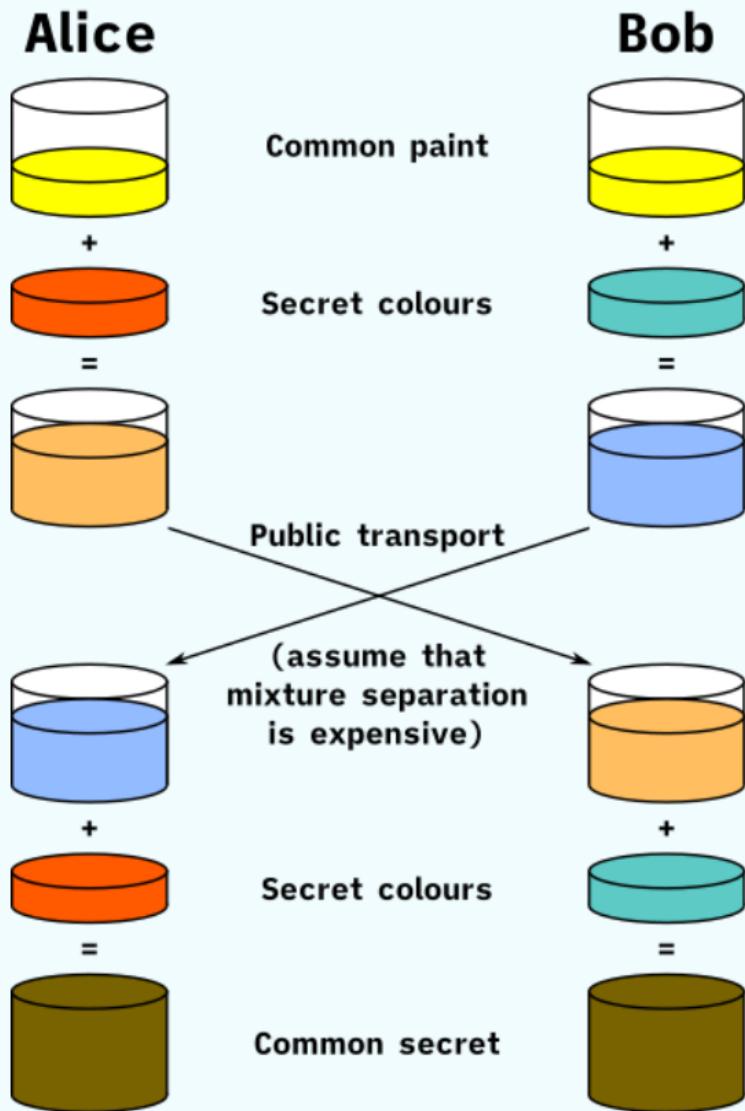
Shared secret



Key Exchange algorithm



Key Exchange Algorithm

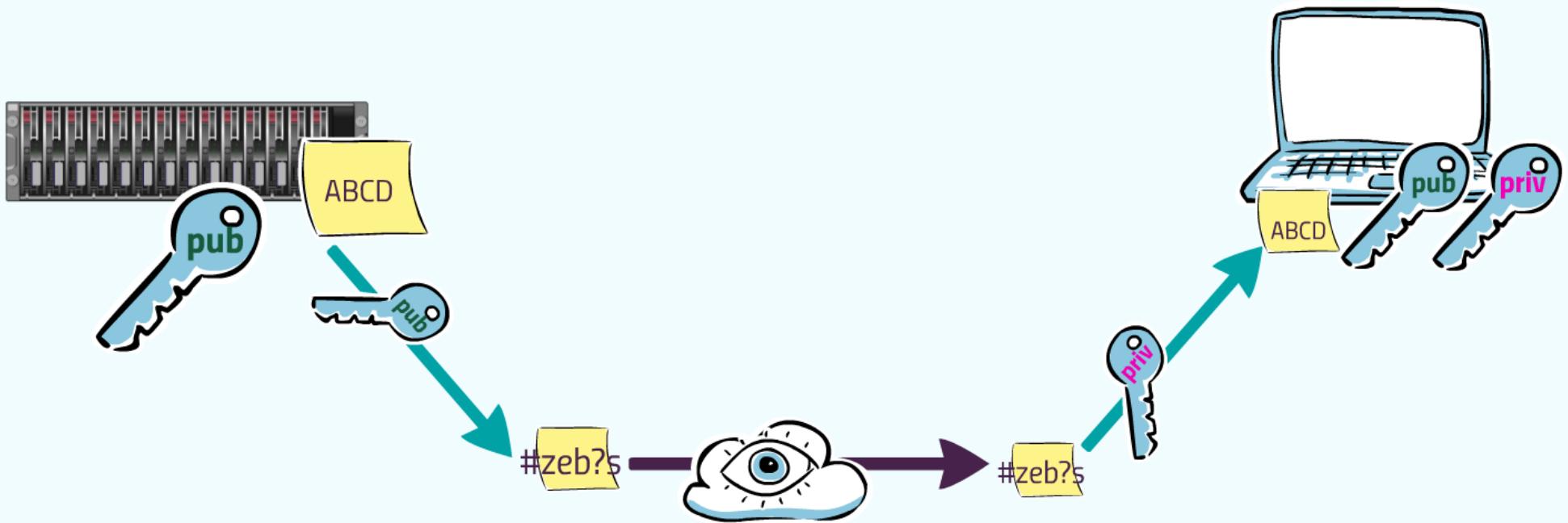


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Source: wikipedia,
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Asymmetric cryptography public/private keys pair

Server and User authentication



IBU HPC Linux cluster

Head node = entry point

ssh binfservms01.unibe.ch

Cent OS 7

2 x 6 cores

64 GB RAM

1 TB /home

10 GBit/s Network uplink



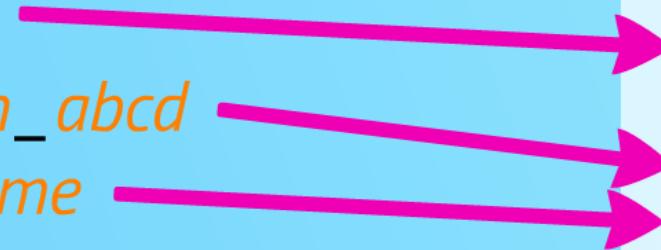
Data Storage

Total active ~ 400 TB

/home/*username*

/data/projects/p*nnn_abcd*

/data/users/*username*



File servers

/home 1 TB

ms01

/data 400 TB

fs07

/scratch

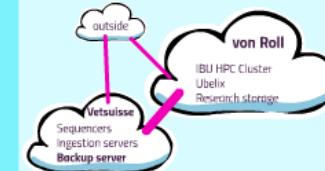
directory local to each node

during job execution: \$SCRATCH

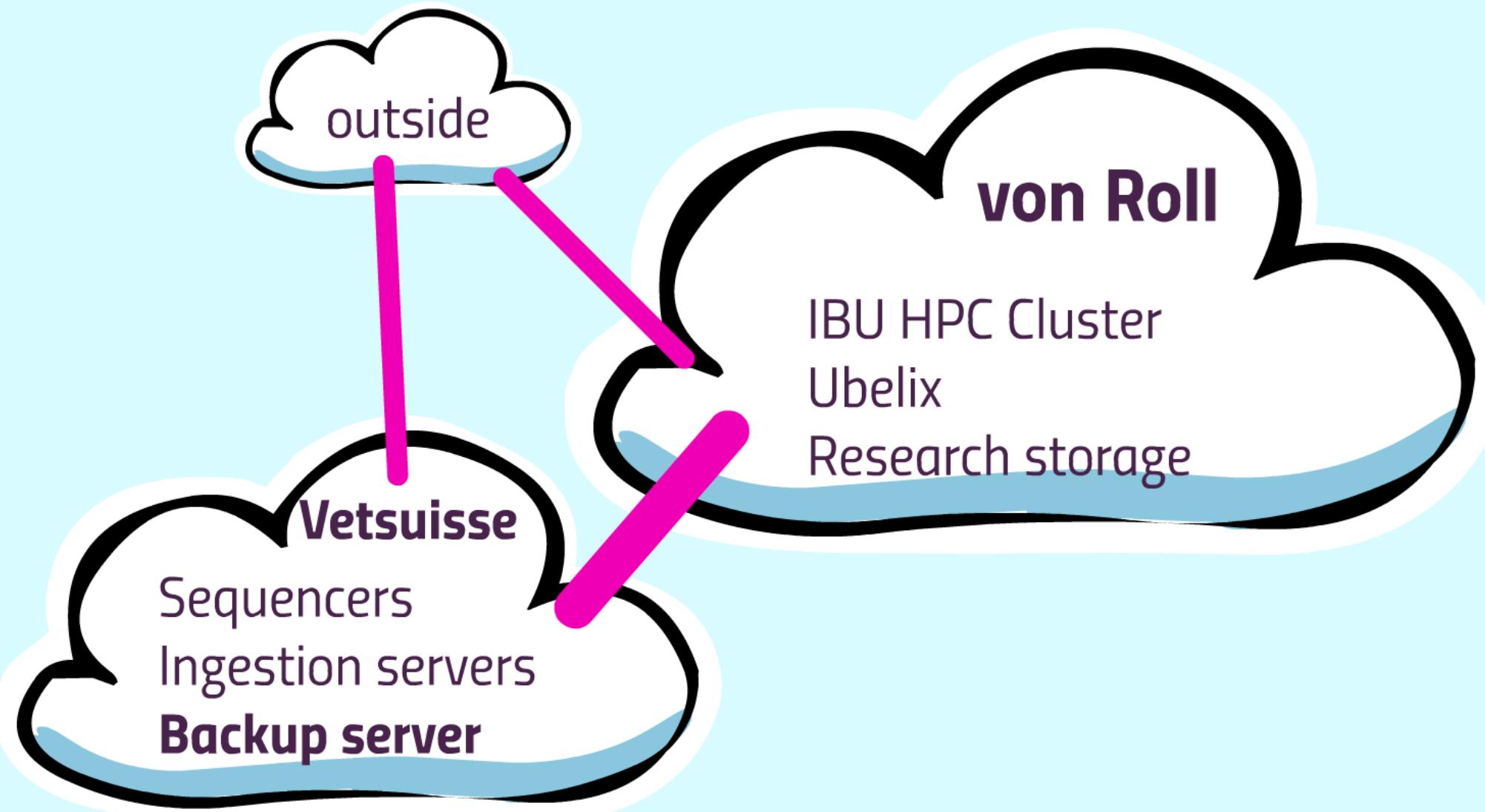
/scratch/172007

deleted after job completion

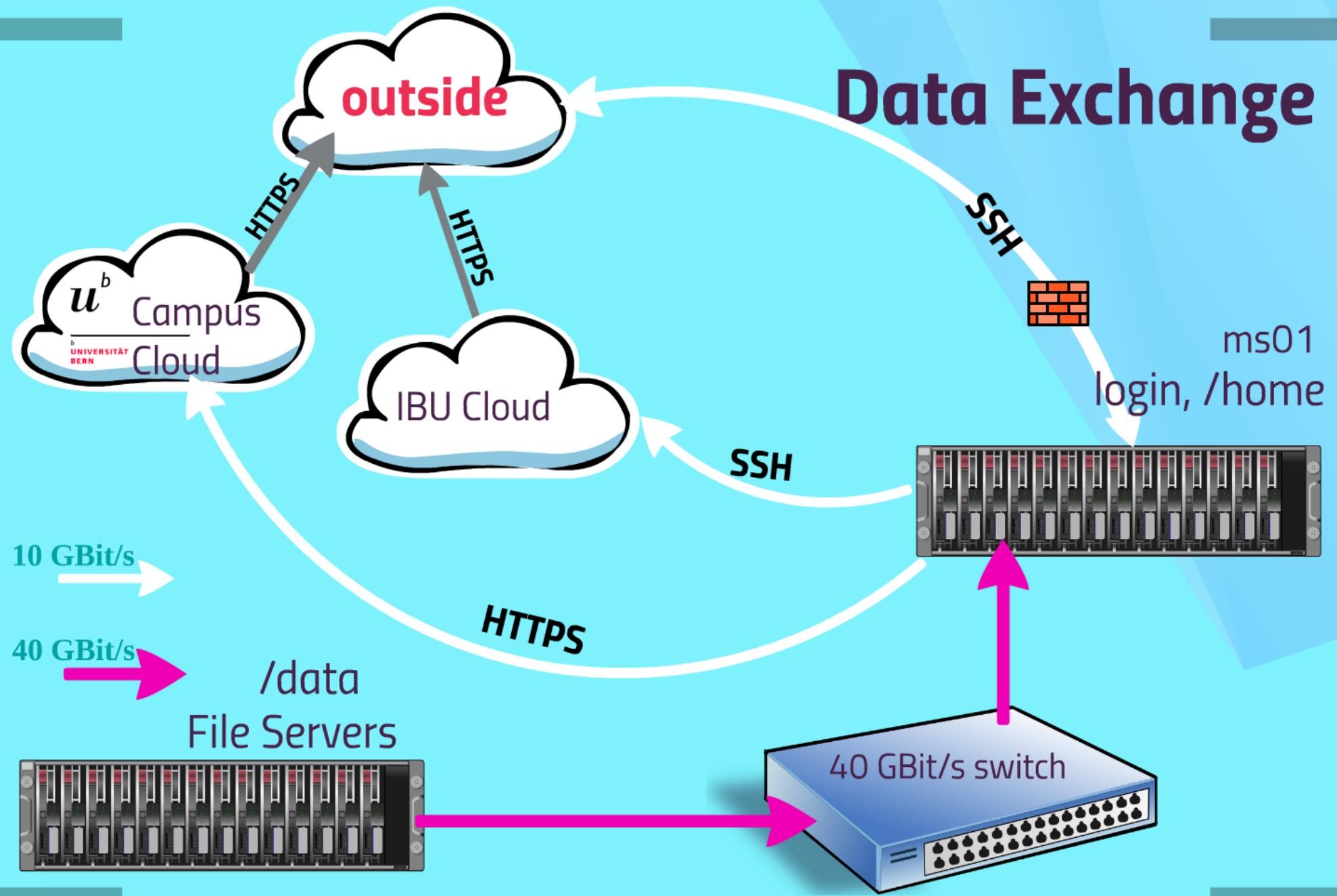
Backup

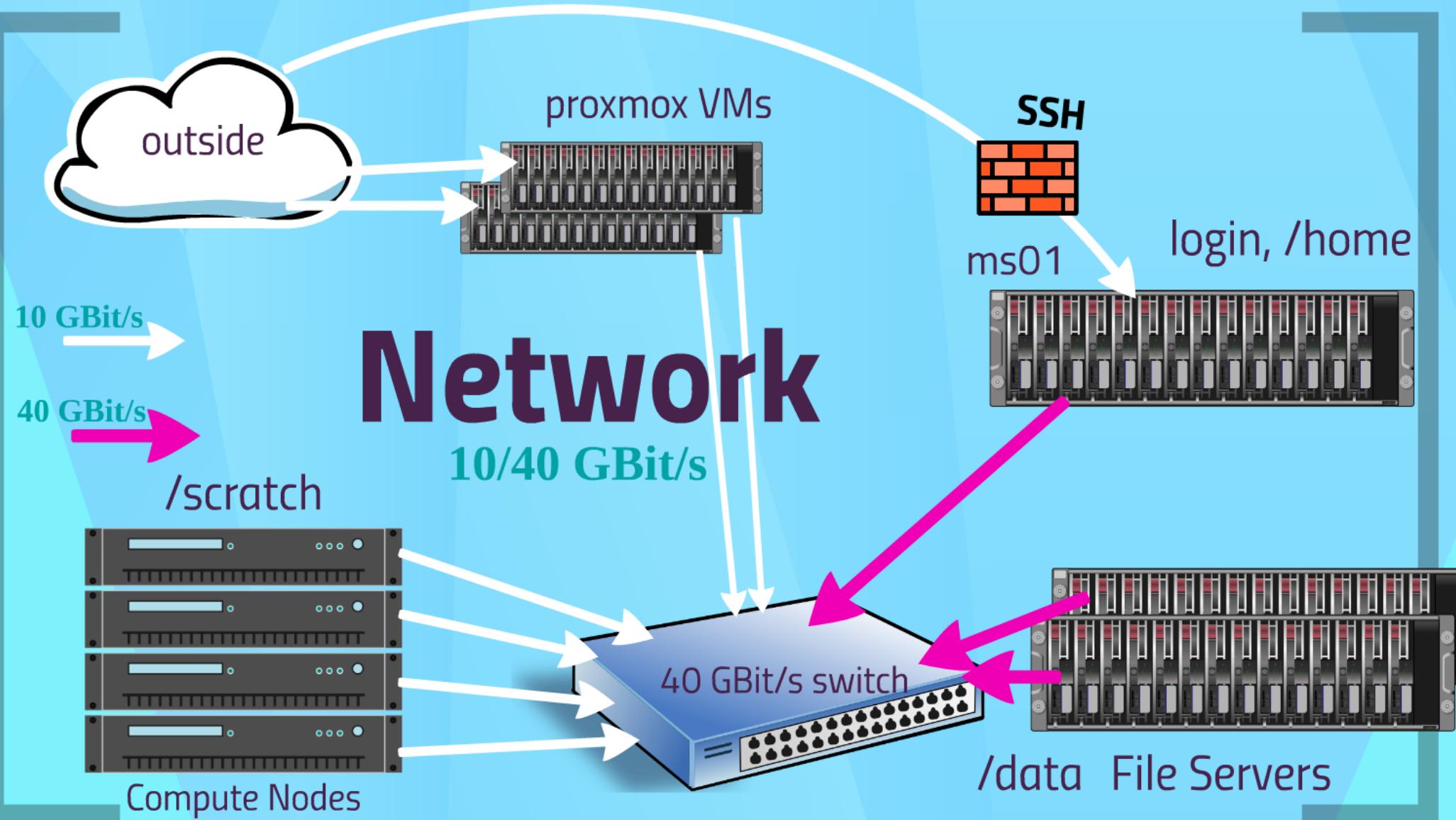


Backup



Data Exchange

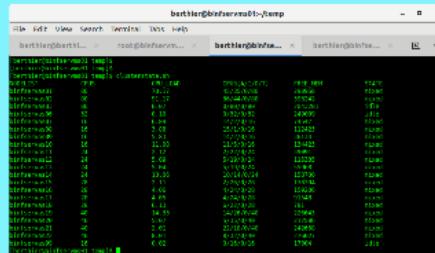




Compute nodes

binfo[01-34]

32 servers, 2048 cores



nodes	#cores	RAM	/scratch
as01-02	80	512G	8TB
as03	80	2T	11TB
as06	32	256G	5TB
as07-10	16	256G	7TB
as11-14	24	256G	11TB
as15-18	28	256G	7TB
as19-26	40	392G	7 - 9TB
as27-30	128	512G	9TB
as31-34	128	512G	3TB

berthier@binfervms01:~/temp

File Edit View Search Terminal Tabs Help

berthier@berthi... ×

root@binfervm... ×

berthier@binfse... ×

berthier@binfse... ×



[berthier@binfervms01 temp]\$

[berthier@binfervms01 temp]\$

[berthier@binfervms01 temp]\$ clusterstate.sh

NODELIST	CPUS	CPU_LOAD	CPUS(A/I/O/T)	FREE_MEM	STATE
binfervas01	80	70.17	45/35/0/80	298958	mixed
binfervas02	80	91.17	36/44/0/80	393242	mixed
binfervas03	80	0.07	0/80/0/80	2043281	idle
binfervas06	32	0.10	0/32/0/32	249009	idle
binfervas07	16	6.89	14/2/0/16	74547	mixed
binfervas08	16	3.88	15/1/0/16	112423	mixed
binfervas09	16	5.83	14/2/0/16	36134	mixed
binfervas10	16	11.08	11/5/0/16	134423	mixed
binfervas11	24	2.12	2/22/0/24	39091	mixed
binfervas12	24	5.09	5/19/0/24	115335	mixed
binfervas13	24	5.04	5/19/0/24	55968	mixed
binfervas14	24	10.06	10/14/0/24	158700	mixed
binfervas15	28	2.11	2/26/0/28	138394	mixed
binfervas16	28	4.06	4/24/0/28	159206	mixed
binfervas17	28	4.05	4/24/0/28	91548	mixed
binfervas18	28	6.13	6/22/0/28	781	mixed
binfervas19	40	14.33	14/26/0/40	226643	mixed
binfervas20	40	5.07	5/35/0/40	212586	mixed
binfervas21	40	2.01	22/18/0/40	242668	mixed
binfervas22	40	8.01	8/32/0/40	276027	mixed
binfervas99	16	0.02	0/16/0/16	17004	idle

[berthier@binfervms01 temp]\$

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File servers

/home 1 TB

ms01

/data 400 TB

fs07

/scratch

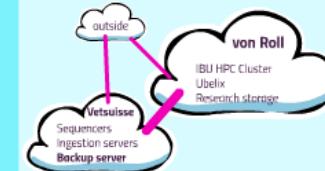
directory local to each node

during job execution: \$SCRATCH

/scratch/172007

deleted after job completion

Backup



/scratch

directory local to each node

during job execution: \$SCRATCH

/scratch/172007

deleted after job completion

Take home



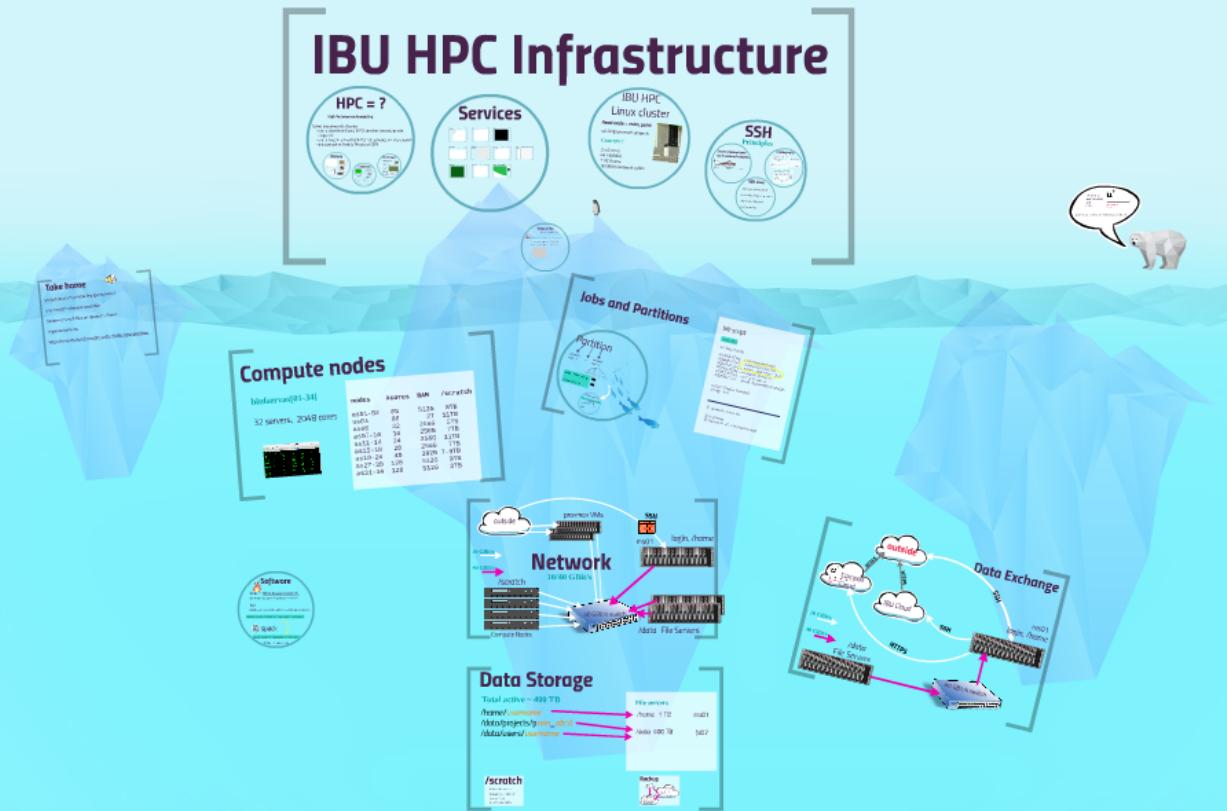
protect your ssh private key (passphrase)

use /scratch whenever possible

beware of small files on /projects, /home

organize backups

<https://projects.bioinformatics.unibe.ch/ibu-best-practices>



Interfaculty Bioinformatics Unit

Pierre Berthier, University of Bern, 26.10.2020