

Interfaculty Bioinformatics Unit

Pierre Berthier, University of Bern, 31.10.2022

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) (High Throughput Computing, HTC): Astrophysics, climate research
- grid computing: Particle Physics at CERN



Services



26 Web Apps

IBU HPC Linux cluster

Head node = entry point

`ssh binfservms01.unibe.ch`

[SSH Tutorial](#)



SSH Principles

Secure channel over an unsecured network

- confidentiality
- integrity
- authentication

Cryptography

Symmetric cryptography
Asymmetric cryptography
public private key pair
User authentication

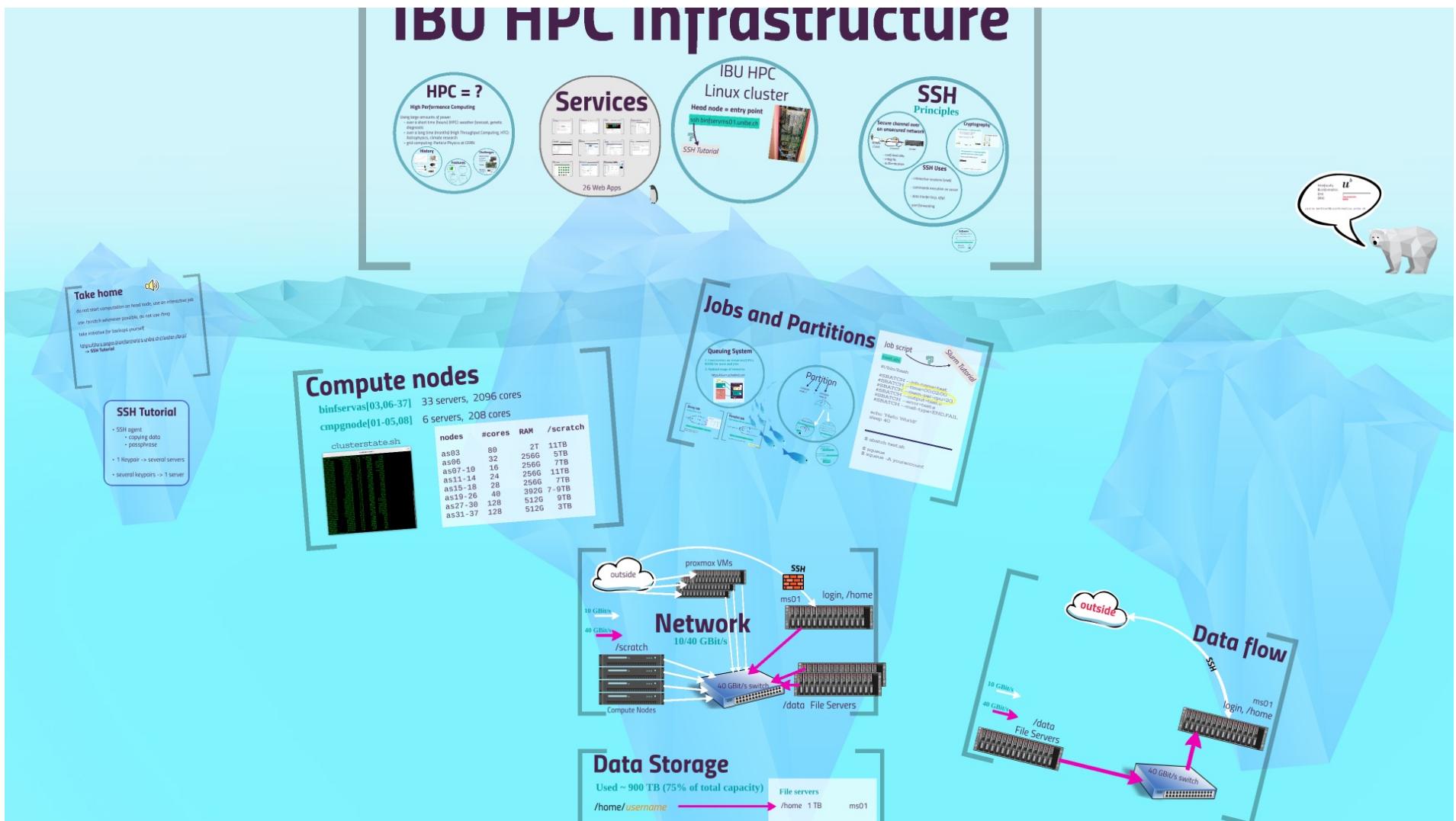
SSH Uses

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



Jobs queue

IBU HPC Infrastructure



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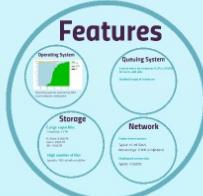
History



Challenges



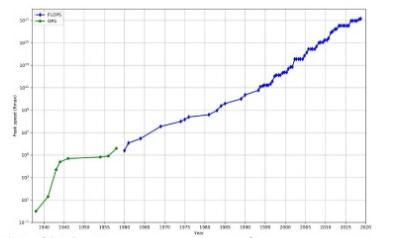
Features



Se



History



Ubelix, 10'000 CPUs



IBU Cluster, 2'000 CPUs

My Laptop, 8 CPUs



Cray-1, 1976, 160 MFLOPS
Smartphone, 2013: 1GFLOPS



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



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

Fee

Operating System



Operating systems used on top 500 supercomputers (wikipedia)

Storage

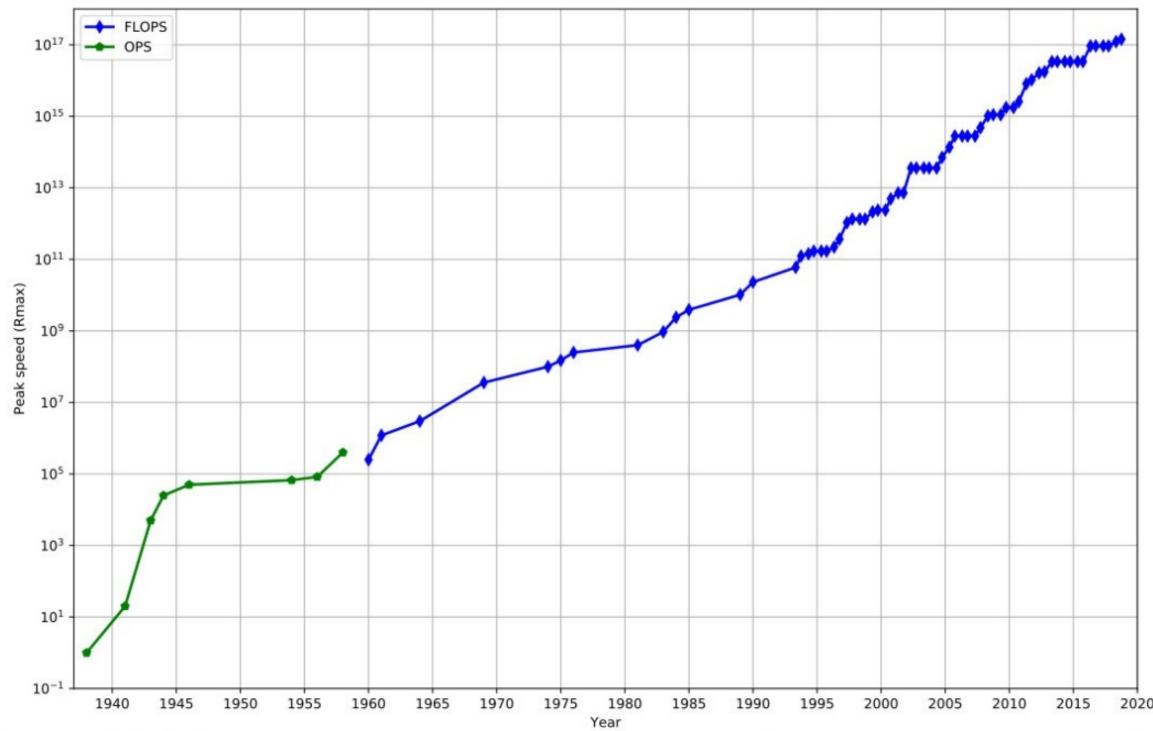
Large capacities

1 Hard Disk: 22 TB

Piz Daint: 8'000 TB

Ubelix: 3'000 TB

IBU-i: 1'000 TR



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

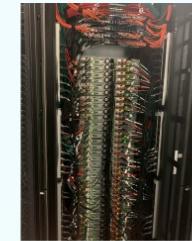


picture: wikipedia



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

Ubelix, 10'000 CPUS



picture: M. Rolli

IBU Cluster, 2'000 CPUs



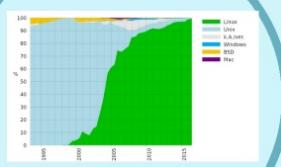
My Laptop, 8 CPUs



Cray
1200

Features

Operating System



Storage

Large capacities

1 Hard Disk: 22 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

Queuing System

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

Optimal usage of resources

Network

Nodes Interconnect

Typical: 10-56 Gbit/s
Network type: TCP/IP or infiniband

Outbound connection

Typical: 10 GBit/s

Piz Daint
IBU: 15 L
My Laptop
City of Bern

Cooling

Data Transfer

IBU Cluster

Uplink: 10 Gbit/s

(10 Gbit/s)



, 160 MFLOPS
2013: 1GFLOPS



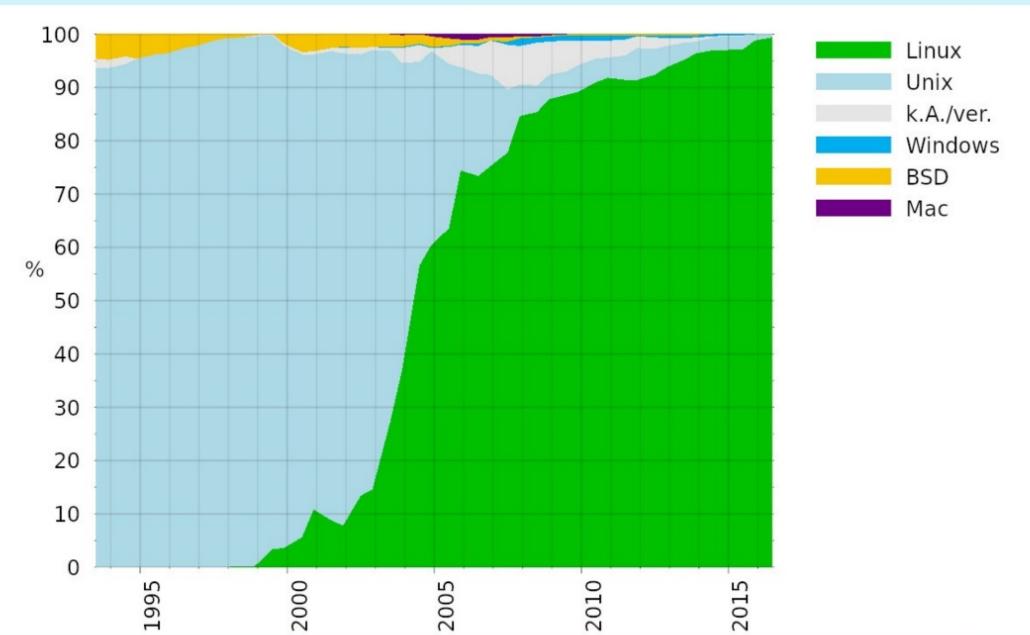
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Uebelix/P, 2007
55'536 CPUs



OPS
(CSCS)

Operating System



Operating systems used on top 500 supercomputers (wikipedia)

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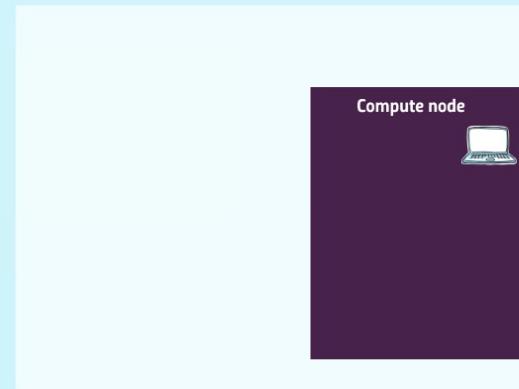
**Concurrency on resources (CPUs, RAM)
for users and jobs**

Optimal usage of resources

Queuing System

Concurrency on resources (CPUs, RAM)
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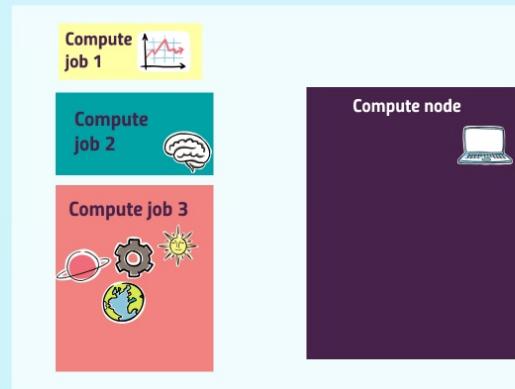
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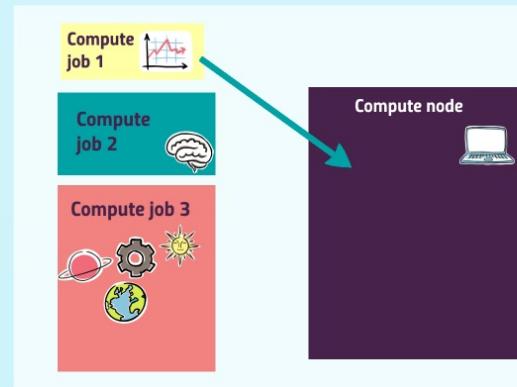
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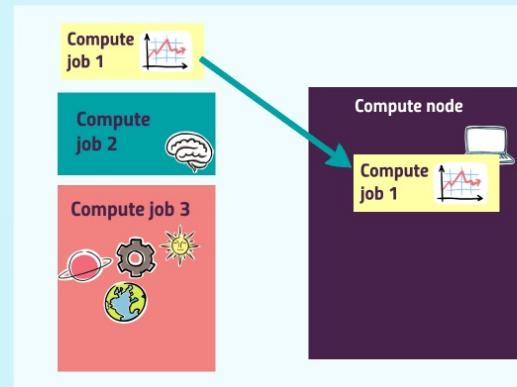
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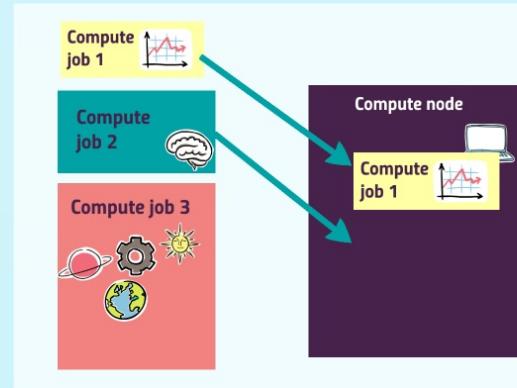
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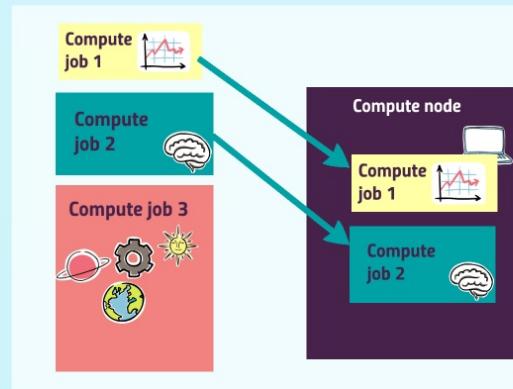
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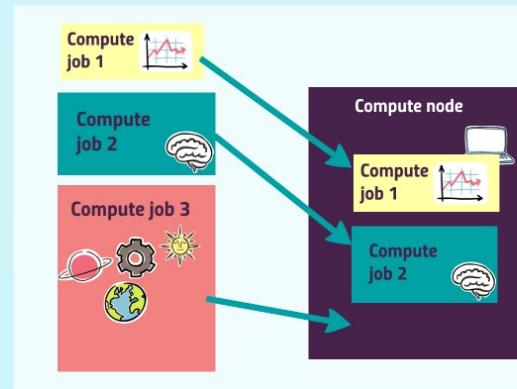
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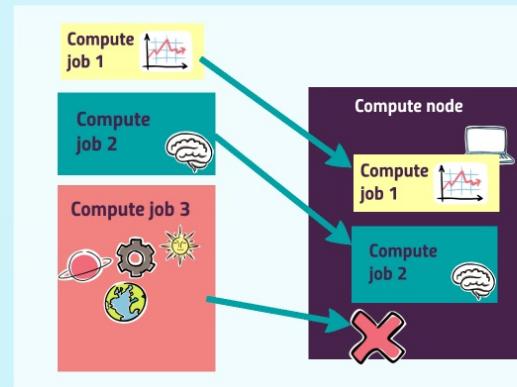
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Storage

Large capacities

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IBU: 1'000 TB

High number of files

typically: 100's of millions of files

Nodes

Typical

Network

Outbox

Typical

Challenges

Electrical Power

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

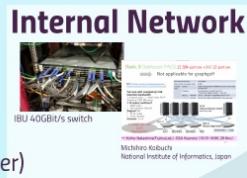


Cooling



Data flow

IBU Cluster: 1 PB Data
Uplink: 10 GBit/s
(10-50 days to transfer)



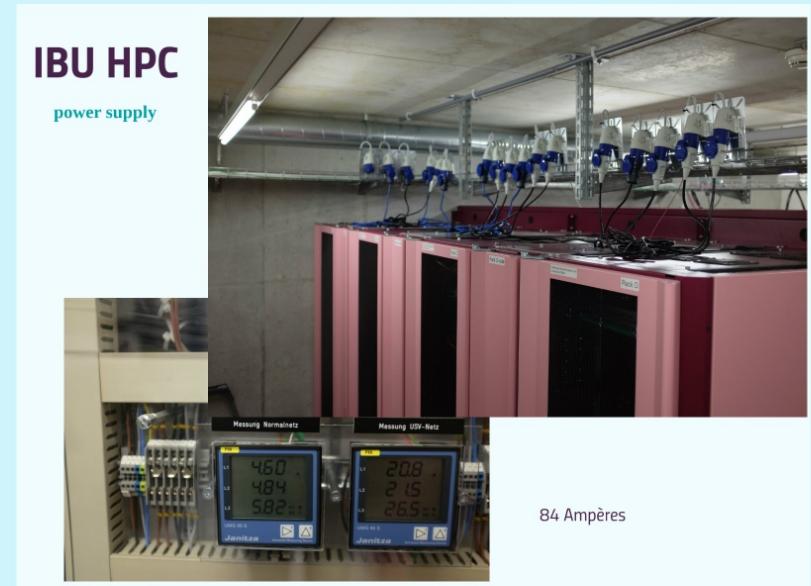
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CSCS cooling

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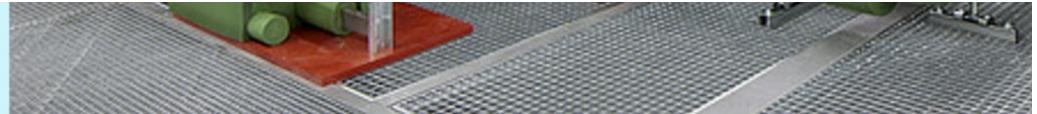
IDU Cluster, 1 PB Data

Internal Network



Data flow

IBU Cluster: 1 PB Data
Uplink: 10 GBit/s
(10-50 days to transfer)



Internal Network



IBU 40Gbit/s switch

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

Not applicable for graphgolf

Total peak performance 24 PFLOPs
Total number of compute nodes 8,219
Compute nodes: 12x 384-port Director Switches (Oakforest-PACS)

Fat-tree with (completely) full-bisection bandwidth

1 compute node = 1 Intel® Xeon® Phi™ Processor (Haswell-EP) + 12x 40GbE ports

of nodes/switches?

• 8208 nodes

• 384 switches (48 port)

Degree? 48

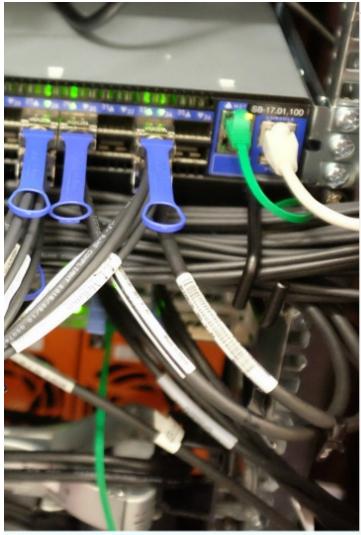
• 24 for network

Diameter: 2 or 4

2 cables per link (Link Aggregation)

→ 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>

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)

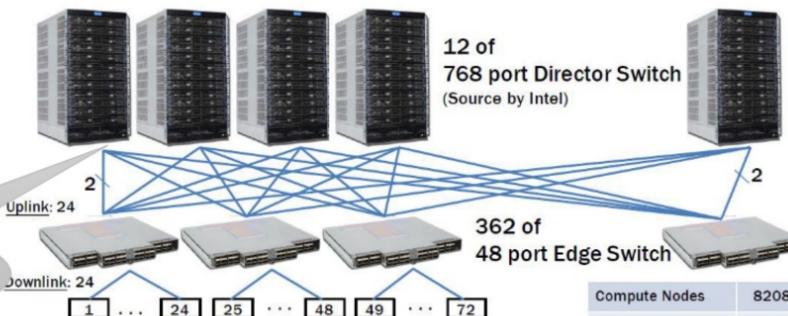
Degree? 48

- 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)

• 11

Michihiro Koibuchi
National Institute of Informatics, Japan

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SSH Tutorial



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Jobs

Services



26 Web Apps



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computing, HTC):

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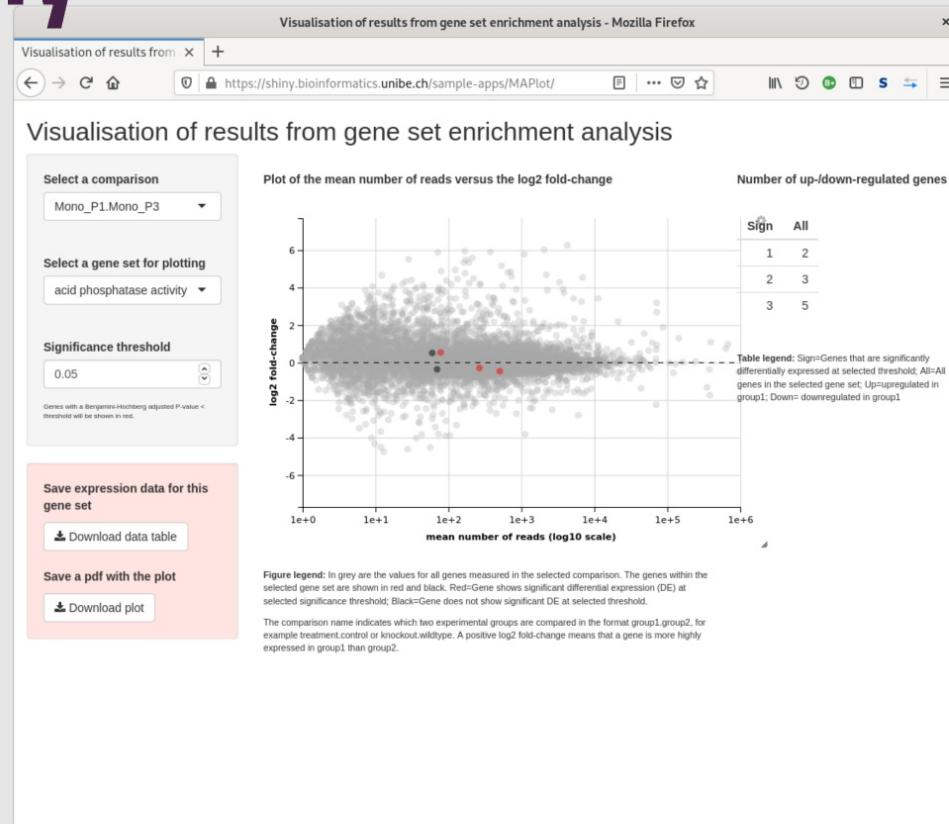


ver

er

Rshiny

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



Sequenceserver

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

The screenshot shows the SequenceServer 1.0.11 web interface. At the top, there is a navigation bar with links for File, Edit, View, History, Bookmarks, Tools, and Help. Below the navigation bar is a toolbar with icons for back, forward, search, and other browser functions. The main content area has a title "SequenceServer 1.0.11" and a "Help & Support" link. A large text input field is labeled "Paste query sequence(s) or drag file containing query sequence(s) in FASTA format here ...". Below this, there is a section titled "Nucleotide databases" containing a list of database names with checkboxes next to them. The databases listed are: 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, and xnt_rna_assembly_all.v1. At the bottom of the interface, there is an "Advanced Parameters:" input field with the placeholder "eg: -evaluate 1.0e-5 -num_alignments 100", a question mark icon, and a blue "BLAST" button.

The screenshot shows a Mozilla Firefox browser window displaying the PACMAN: PACbio Methylation ANalyzer website at <https://bugfri.unibe.ch/>. The page features a header with the University of Freiburg logo and navigation links for HOME, MSC BIOINFORMATICS, SEMINAR, RESEARCH, and ABOUT US. A large, stylized illustration of the video game character Pac-Man and three ghostly enemies (blue, green, and pink) is centered on the page. Below the illustration, a section titled "Limitations" contains the following bullet points:

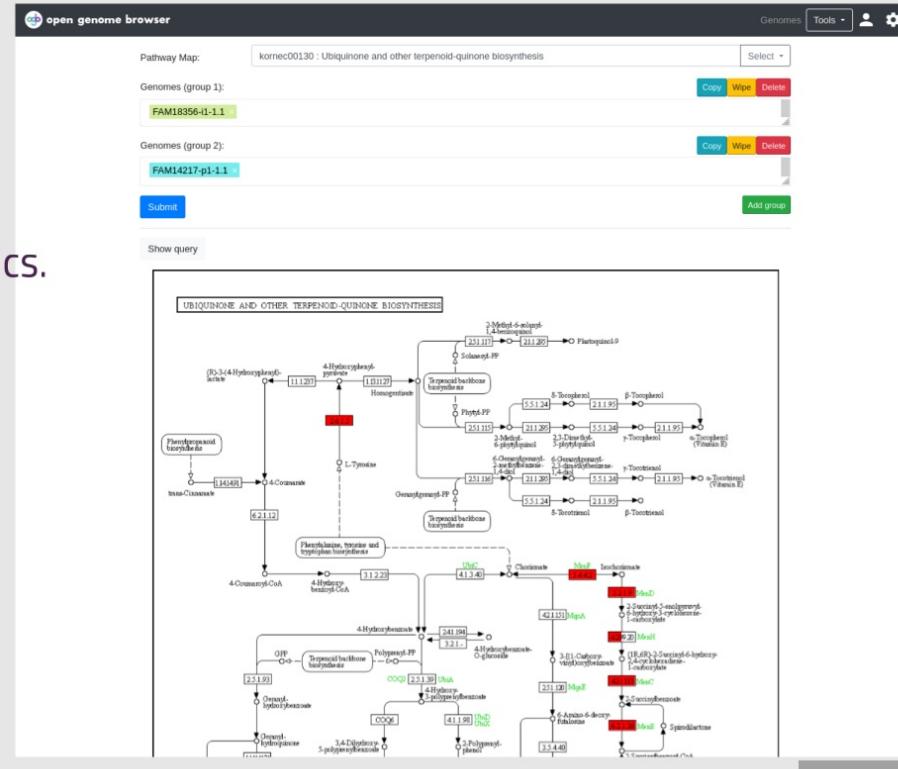
- The **contigs** smaller than 10'000bp are ignored.
- The **step** cannot be smaller than 500bp
- The **window** must be bigger than the step
- Maximum **4 motifs** are represented
- **GFF** headers must correspond to **FASTA** headers

On the right side of the page, there is a section titled "PACMAN" with the subtitle "PACific biosciences Methylation ANalyzer". It describes the web server's function: "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." Below this text, there are two input fields: "Input" (labeled "FASTA (genome) ([example](#))" and "motifs.gff (Pacbio output) ([example](#))") and two "Browse..." buttons. The first button has the message "No file selected." and the second also has "No file selected."

OpenGenomeBrowser

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

web platform for
comparative genomics.



openBIS

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

The screenshot shows the openBIS web application interface. At the top, there is a navigation bar with a search bar labeled "Global". Below the navigation bar, the title "Bbb: TEST1" is displayed. On the left side, there is a sidebar titled "Datasets" containing a list of datasets: Bruggmann, David Test, Default, Public, Yvesn, Project Test1, and TEST1. Under TEST1, two entries are listed: 20181211162058314-30 and 20181211162058314-31. The main content area has sections for "Process all comparisons" with a "Start processing" button, "Pick groups to compare" with dropdown menus for "Group by", "Group 1", and "Group 2", and a "Metadata" section. The "Metadata" section displays the following details:

- Group:** IBU_University of Bern
- Analysis:** RNA-Seq
- Species:** Homo Sapiens
- Platform:** Illumina HiSeq 2000

At the bottom of the screen, a Windows taskbar is visible with various icons and system status indicators.

Galaxy

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

The screenshot shows the Galaxy web interface running in Mozilla Firefox. The title bar reads "Galaxy - Mozilla Firefox". The address bar shows the URL "https://galaxy.bioinformatics.unibe.ch". The main content area displays a "Hello, Galaxy is running!" message with links to "Configuring Galaxy" and "Installing Tools". To the left is a sidebar titled "Tools" with a search bar and a list of 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, there is a "History" section titled "Unnamed history" which is currently empty.

Gitlab

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

The screenshot shows a Mozilla Firefox browser window displaying a GitLab project. 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 shows the project navigation menu:

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

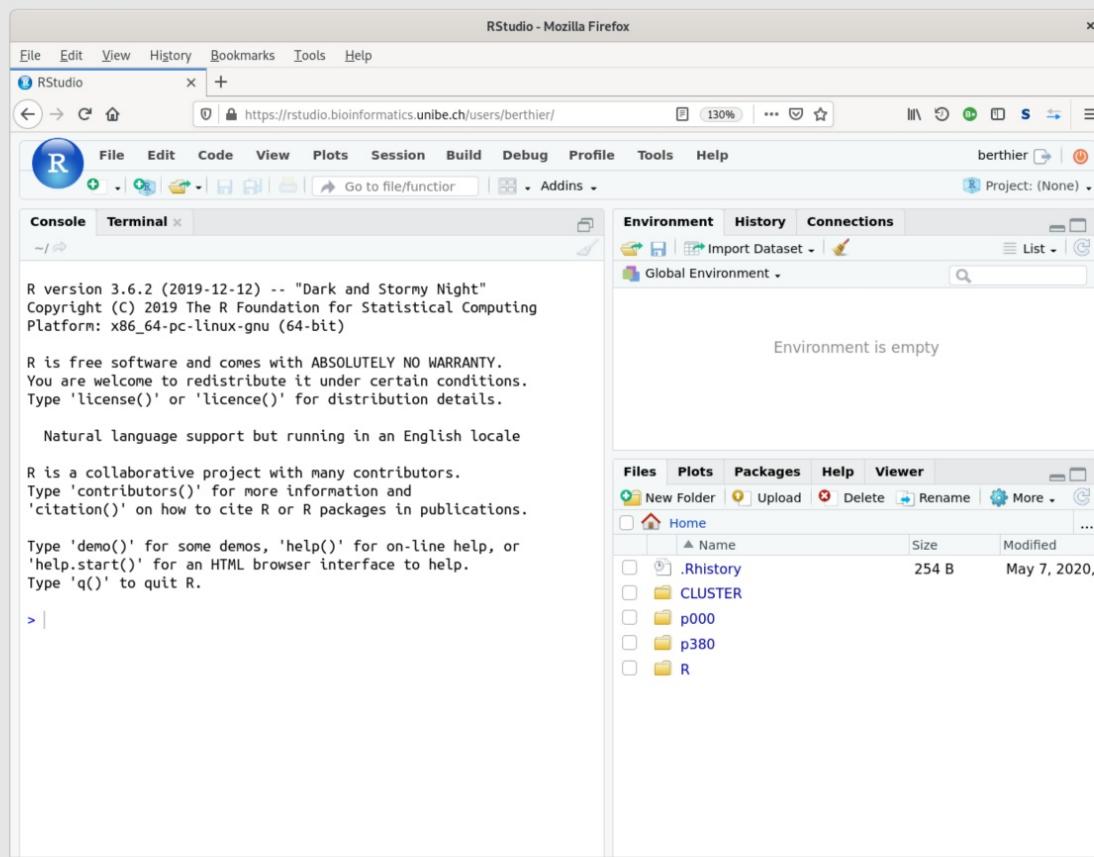
The main content area displays the project details for "spack IBU repos" (Project ID: 11). It includes the following information:

- Statistics: ~ 12 Commits, 1 Branch, 0 Tags, 625 KB Files.
- Description: Spack Repository for IBU specific packages.
- Recent commit: "new package py-mg-toolkit and dependencies" by Pierre Berthier, 2 months ago, commit 5fe3f9dc.
- Buttons for README, Add LICENSE, Add CHANGELOG, Add CONTRIBUTING, Enable Auto DevOps, Add Kubernetes cluster, and Set up CI/CD.
- A table showing the last commits:

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

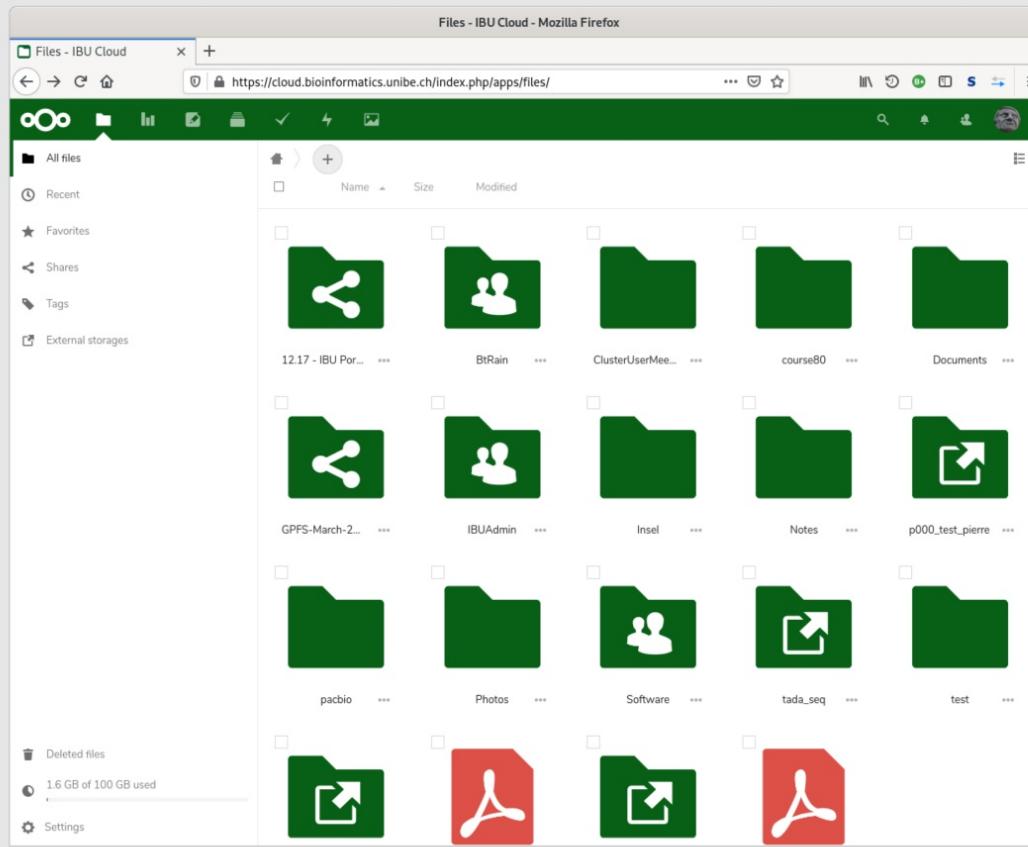
Rstudio

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



IBU Cloud

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



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

The screenshot shows the 'IBU Projects' instance of the OpenProject software. The interface is divided into several sections:

- Header:** Shows the title 'IBU Projects - Mozilla Firefox' and the URL 'https://projects.bioinformatics.unibe.ch/'.
- Welcome Section:** Contains a 'WELCOME!' message, a brief description of the tool, and links to the Bioinformatics Unit website and a new project creation page.
- Projects Section:** Displays a list of newest visible projects:
 - p532 Plant root bacteria genomes [3 TB] (01.09.2020)
 - p532 BX-rhizosphere-metagenomics [1 TB] (30.04.2020)
 - p531 Felis Catus whole genome Analysis [10 TB] (29.04.2020)

Buttons for '+ Project' and 'View all projects' are present.
- New Features Section:** Lists various improvements and includes a 'Learn more about the new features' link and a small icon representing a dashboard or board.
- Users Section:** Shows the newest registered users:
 - Chantal Bachmann (05.05.2020)
 - Marco Kreuzer (01.05.2020)
 - Irene Adrian-Kalchhauser (26.04.2020)

A '+ Invite user' button is available.
- My Account Section:** Provides links to 'Profile' and 'My page'.
- OpenProject Community Section:** Includes links to 'User guides' and 'Shortcuts'.

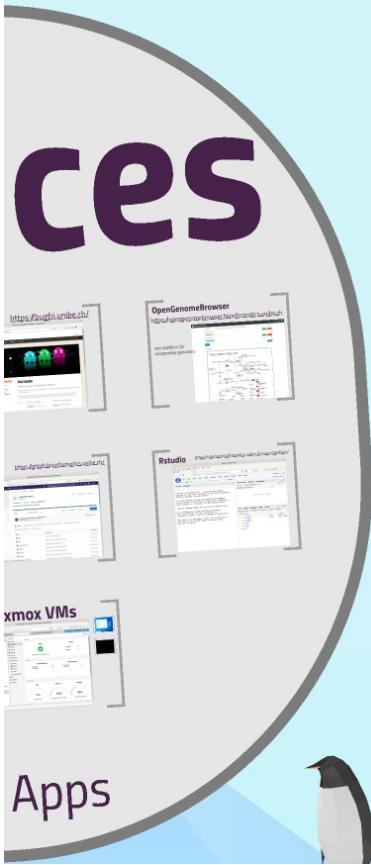
IBU HPC Linux cluster

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SSH Tutorial



SSH

Principles

Secure channel over
an unsecured network



- confidentiality
- integrity
- authentication

SSH Uses

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

Cryptography

Symmetric cryptography

Goal: establish a secured channel
=> confidentiality+integrity
Needs a Shared Secret.



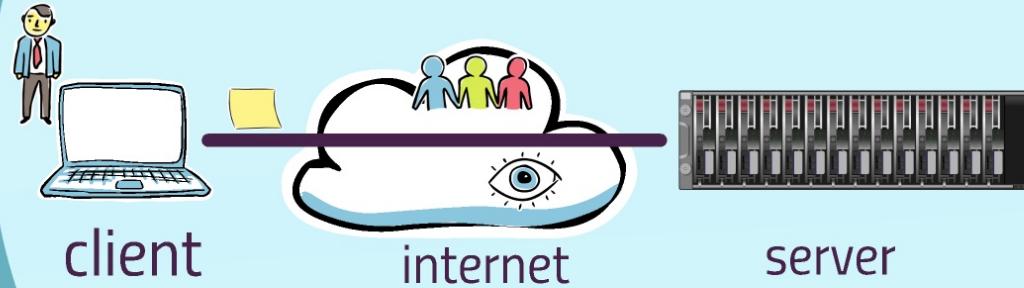
Asymmetric cryptography public/private keys pair

User authentication



Server authentication: same principle, reverse sides

Secure channel over an unsecured network



- confidentiality
- integrity
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SSH Uses

- integrity
- authentication

SSH Uses

Server authentication: same principle, reverse sides

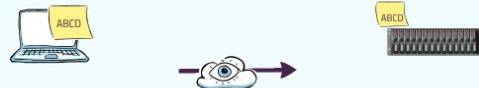
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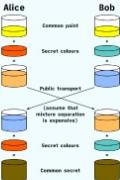
Symmetric cryptography

Goal: establish a secured channel
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Needs a Shared Secret:



Key Exchange Algorithm



Asymmetric cryptography public/private keys pair

User authentication



Server authentication: same principle, reverse sides

SSH Uses

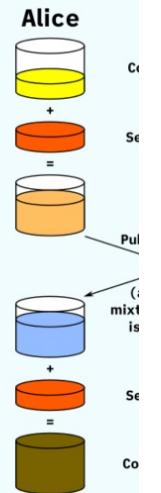
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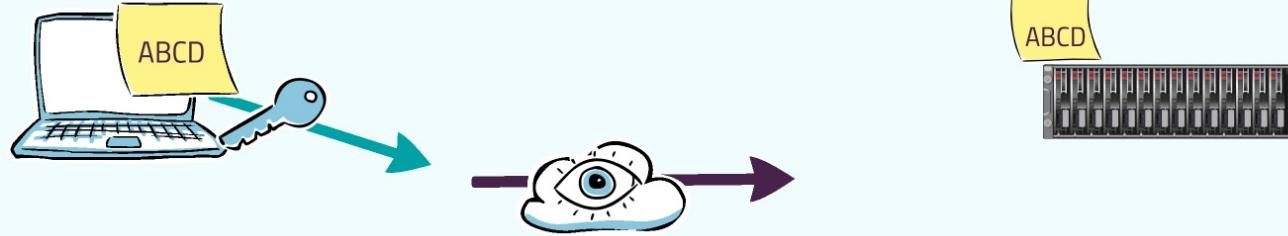
Key



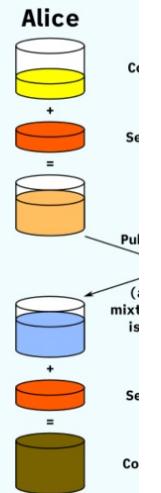
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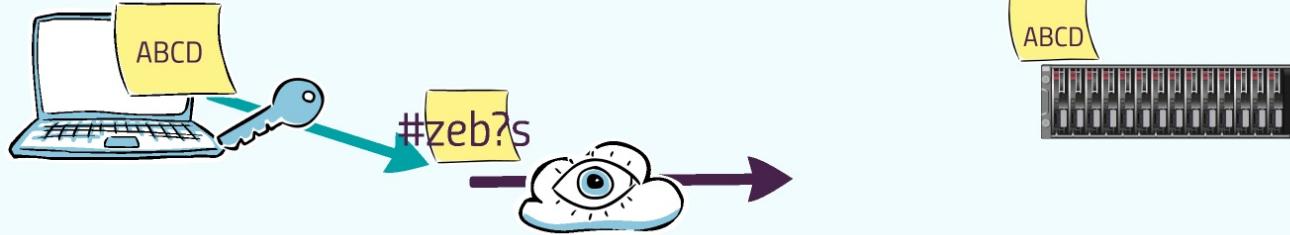
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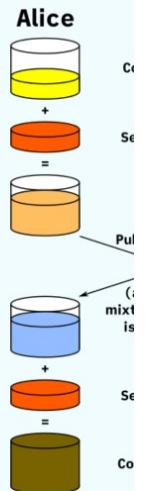
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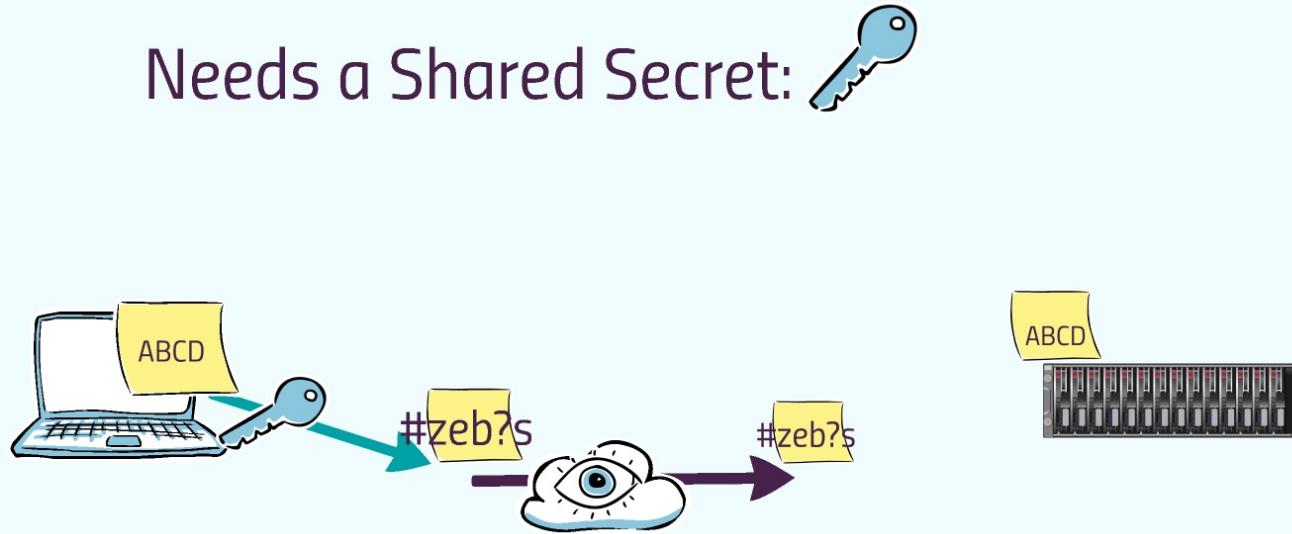
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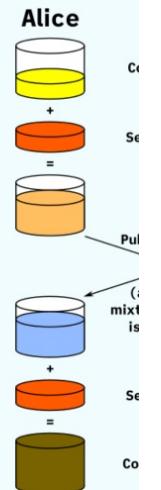
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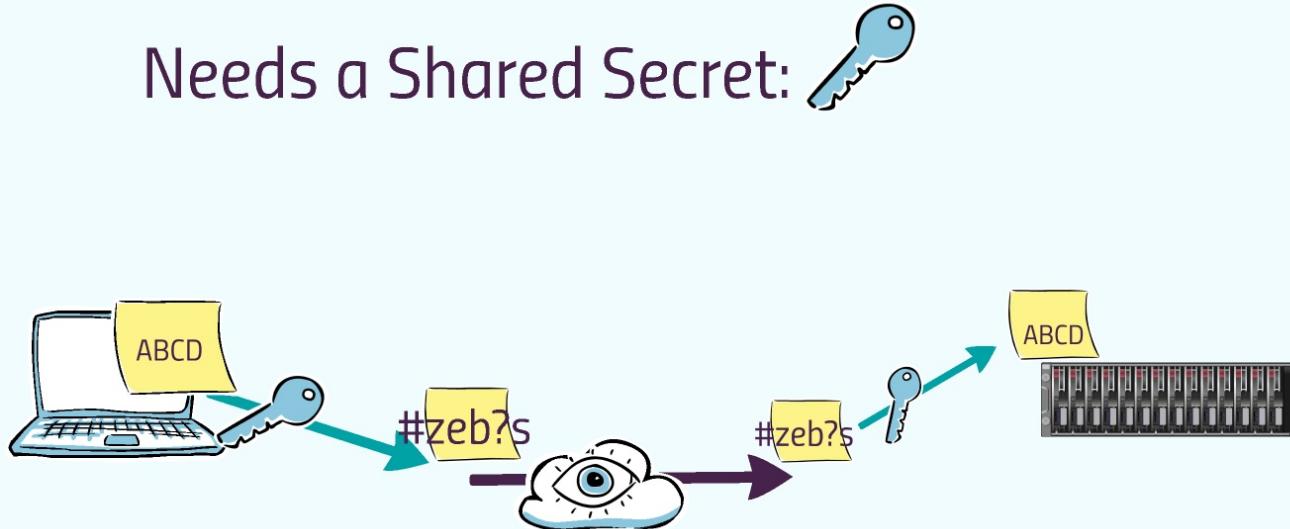
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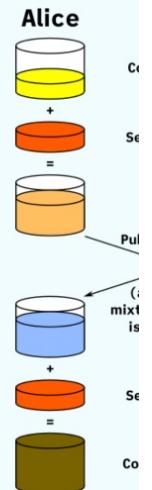
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Needs a Shared Secret:



Key



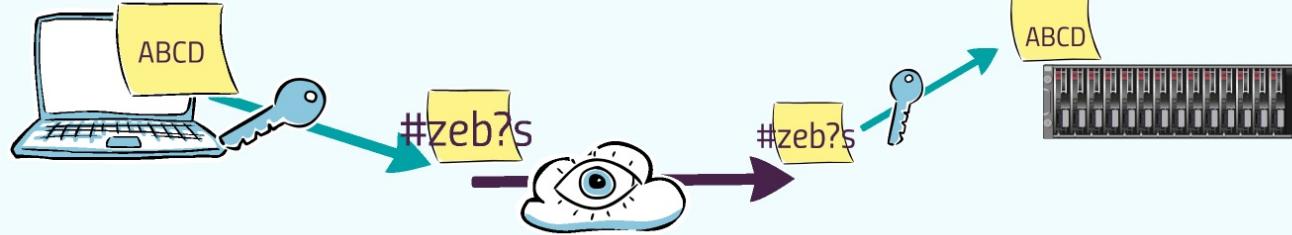
Symmetric cryptography

Goal: establish a secured channel
=> confidentiality+integrity

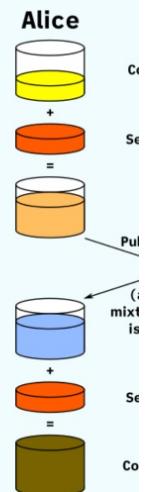
Needs a Shared Secret:



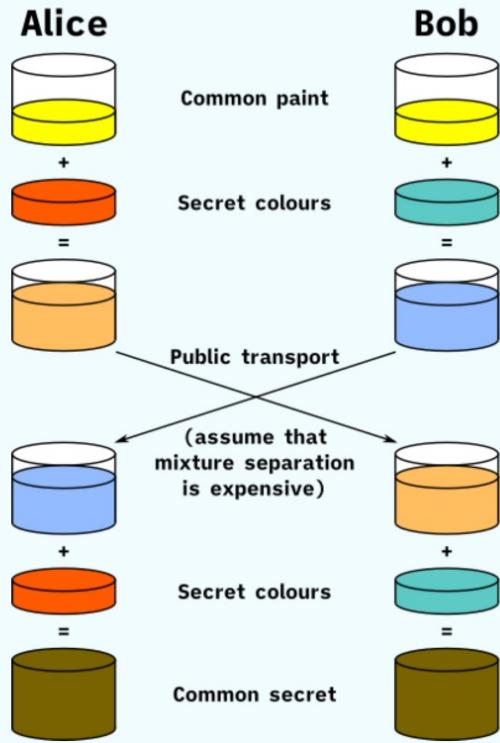
=> needs a Key Exchange Algorithm



Key



Key Exchange Algorithm



Asymmetric cryptography public/private keys pair

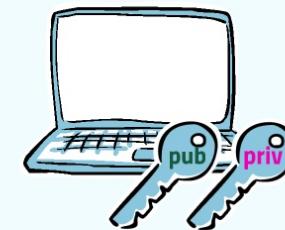
User authentication



Server authentication: same principle, reverse sides

Asymmetric cryptography public/private keys pair

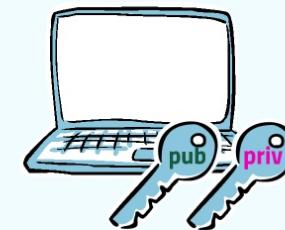
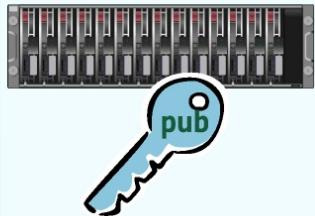
User authentication



Server authentication: same principle, reverse sides

Asymmetric cryptography public/private keys pair

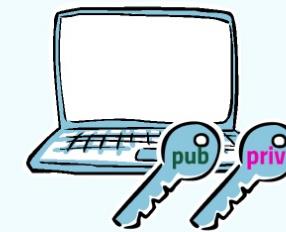
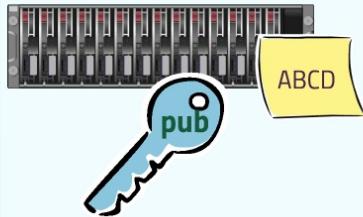
User authentication



Server authentication: same principle, reverse sides

Asymmetric cryptography public/private keys pair

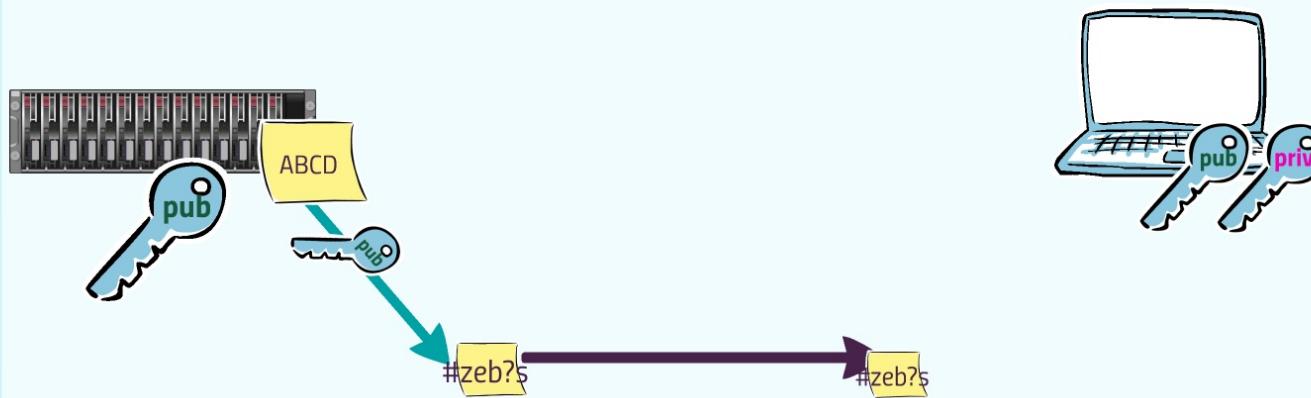
User authentication



Server authentication: same principle, reverse sides

Asymmetric cryptography public/private keys pair

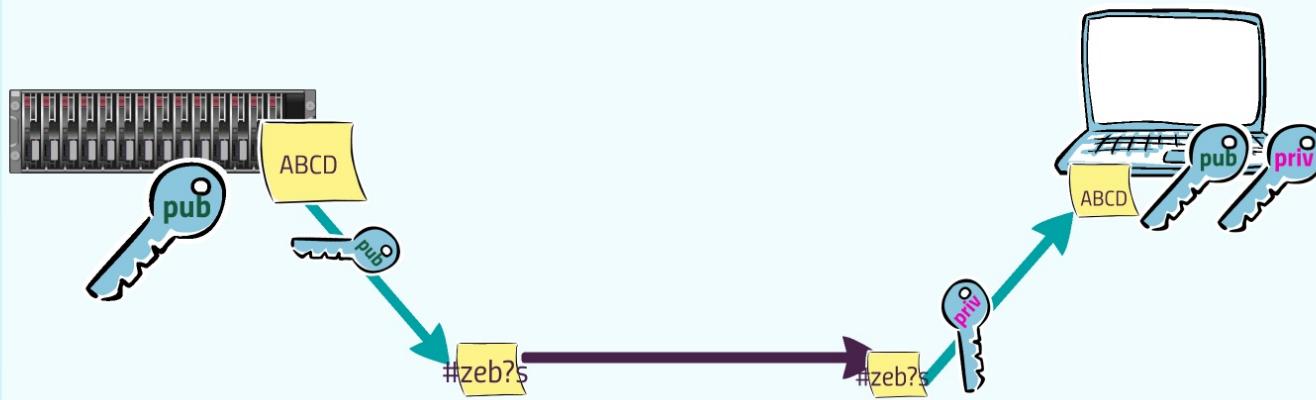
User authentication



Server authentication: same principle, reverse sides

Asymmetric cryptography public/private keys pair

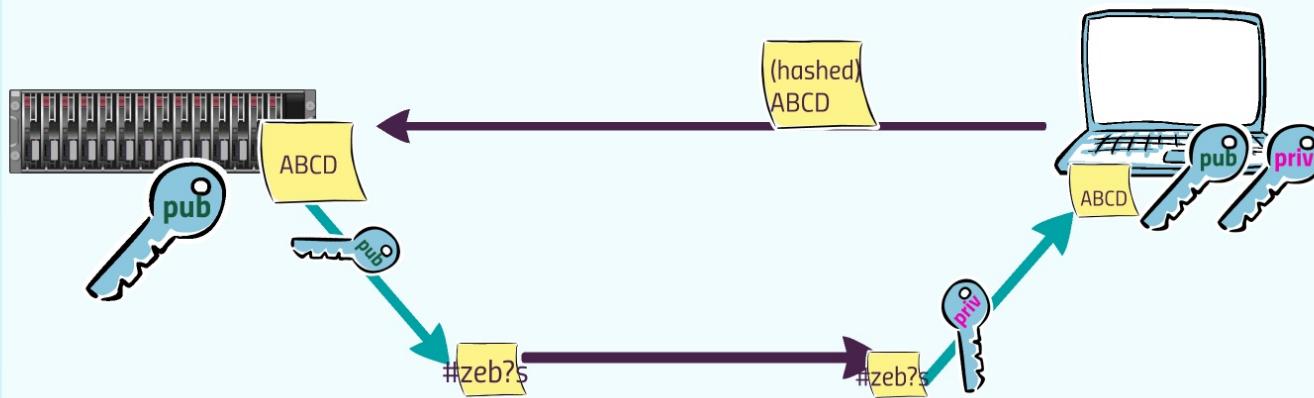
User authentication



Server authentication: same principle, reverse sides

Asymmetric cryptography public/private keys pair

User authentication



Server authentication: same principle, reverse sides

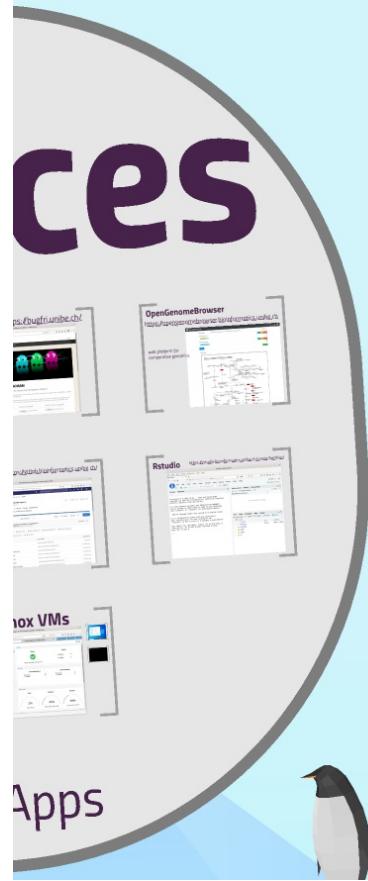
IBU HPC Linux cluster

Head node = entry point

`ssh binfservms01.unibe.ch`



SSH Tutorial



IBU HPC Linux cluster

Head node = entry point

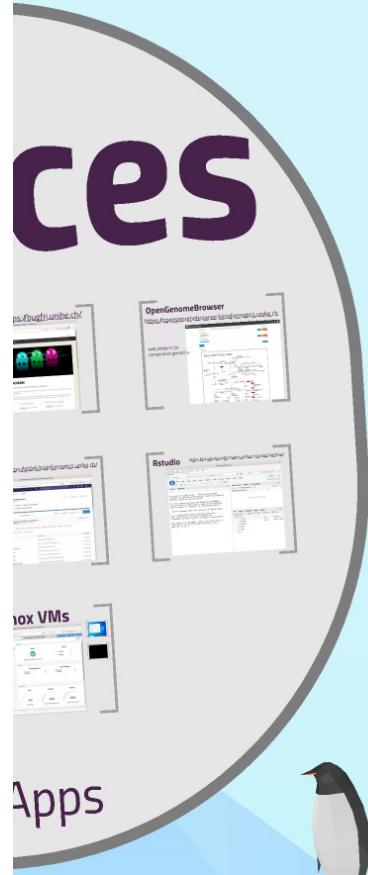
`ssh binfservms01.unibe.ch`



SSH Tutorial



Cent OS 7



IBU HPC Linux cluster

Head node = entry point

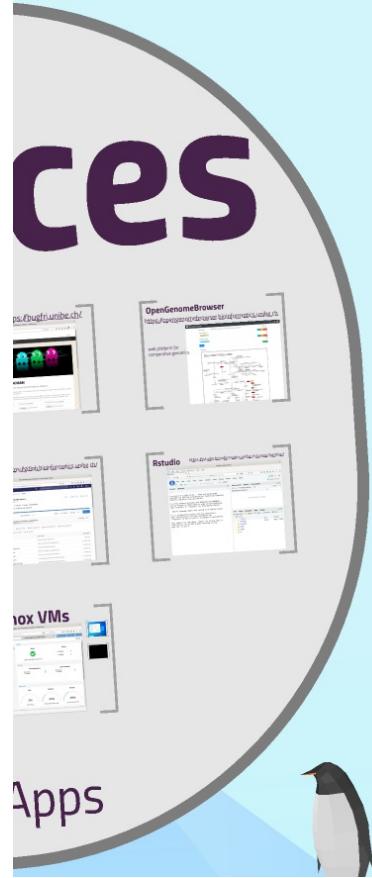
`ssh binfservms01.unibe.ch`



SSH Tutorial

Cent OS 7

10 GBit/s Network uplink
12 CPU cores
64 GB RAM
1 TB /home



Compute nodes

binfoervas[03,06-37]

33 servers, 2096 cores

cmpgnode[01-05,08]

6 servers, 208 cores

clusterstate.sh

```
root@binfoervas01 ~]# clusterstate.sh
NODELIST          CPUs(A/I/O/T)   CPU_LOAD    FREEMEMORY      STATE
binfoervas03      20/60/0/00     20.66       1844352      mixed
binfoervas04      2/30/0/00      0.01        45268       mixed
binfoervas05      15/30/0/00     0.01        518352      allocated
binfoervas06      16/0/0/16      5.87       1623668      allocated
binfoervas07      16/0/0/16      2.73       242832      allocated
binfoervas08      16/0/0/16      1.01       112385      allocated
binfoervas09      16/0/0/16      1.79       242832      allocated
binfoervas10      16/0/0/16      2.82       46224       allocated
binfoervas11      16/0/0/16      1.79       242832      mixed
binfoervas12      24/0/0/24      2.82       46224       allocated
binfoervas13      16/0/0/24      1.79       242832      mixed
binfoervas14      15/30/0/24     24.17       41368       mixed
binfoervas15      17/11/0/28     1.81       238544      mixed
binfoervas16      24/4/0/28      88.95      111768      mixed
binfoervas17      16/0/0/28      1.81       238544      mixed
binfoervas18      9/28/0/28      0.43       112385      idle
binfoervas19      33/7/0/48      4.60       335184      mixed
binfoervas20      33/7/0/48      4.47       335184      mixed
binfoervas21      33/7/0/48      4.47       335184      mixed
binfoervas22      32/8/0/48      2.96       355664      mixed
binfoervas23      32/8/0/48      3.54       355664      mixed
binfoervas24      32/8/0/48      3.54       355664      mixed
binfoervas25      32/8/0/48      3.83       355664      mixed
binfoervas26      32/8/0/48      4.24       355664      mixed
binfoervas27      0/0/120/128    0.01       512800      down*
binfoervas28      128/0/0/128    0.01       512800      allocated
binfoervas29      128/0/0/128    4.76       376832      allocated
binfoervas30      120/0/0/128    0.01       20480      mixed
binfoervas31      128/0/0/128    0.01       175000      idle
binfoervas32      128/0/0/128    3.74       481664      allocated
binfoervas33      128/0/0/128    8.87       428169      allocated
binfoervas34      128/0/0/128    12.34      454656      allocated
binfoervas35      128/0/0/128    58.01      153600      allocated
binfoervas36      128/0/0/128    0.63       401664      allocated
binfoervas37      127/1/0/128    45.36      215168      mixed
binfoervas39      0/0/0/0       0.01       175000      idle
cpgnode01         0/16/0/16     0.01       175000      idle
cpgnode02         0/32/0/32     0.01       175000      idle
cpgnode03         0/20/0/20     0.01       145000      idle
cpgnode04         0/10/0/20     0.01       115000      idle
cpgnode05         0/38/0/36     0.01       210000      idle
cpgnode06         0/12/0/12     0.01       32768      idle
cpgnode07         0/12/0/12     0.01       32768      idle
```

nodes	#cores	RAM	/scratch
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
as31-37	128	512G	3TB

clusterstate.sh

```
[root@binfservms01 ~]# clusterstate.sh
NODELIST      CPUS(A/I/O/T)    CPU_LOAD    FREEMEMORY      STATE
binfservas03   20/60/0/80     20.06       1844352      mixed
binfservas06   2/30/0/32      0.07        45200       mixed
binfservas07   16/0/0/16      2.30        242832      allocated
binfservas08   16/0/0/16      5.87        162960      allocated
binfservas09   16/0/0/16      2.73        242832      allocated
binfservas10   16/0/0/16      1.51        242832      allocated
binfservas11   16/8/0/24      1.79        242832      mixed
binfservas12   24/0/0/24      2.82        46224       allocated
binfservas13   16/8/0/24      1.70        242832      mixed
binfservas14   19/5/0/24      24.17       41104       mixed
binfservas15   17/11/0/28     1.84        230544      mixed
binfservas16   24/4/0/28      80.95       111760      mixed
binfservas17   16/12/0/28     2.51        242832      mixed
binfservas18   0/28/0/28      0.43        112385      idle
binfservas19   33/7/0/40      4.60        335184      mixed
binfservas20   33/7/0/40      4.45        335184      mixed
binfservas21   32/8/0/40      3.02        355664      mixed
binfservas22   32/8/0/40      2.96        355664      mixed
binfservas23   32/8/0/40      3.54        355664      mixed
binfservas24   32/8/0/40      3.34        355664      mixed
binfservas25   32/8/0/40      3.83        355664      mixed
binfservas26   32/8/0/40      4.26        355664      mixed
binfservas27   0/0/128/128    0.01        512000      down*
binfservas28   128/0/0/128    5.57       401664      allocated
binfservas29   128/0/0/128    4.76       376832      allocated
binfservas30   120/8/0/128    0.01        20480       mixed
binfservas31   128/0/0/128    5.01       401664      allocated
binfservas32   128/0/0/128    5.74       401664      allocated
binfservas33   128/0/0/128    8.87       428160      allocated
binfservas34   128/0/0/128    12.34      454656      allocated
binfservas35   128/0/0/128    50.34      6392        allocated
binfservas36   128/0/0/128    6.63       401664      allocated
binfservas37   127/1/0/128    45.36      215168      mixed
binfservas99   0/8/0/8       0.01        1800        idle
cmpgnode01    0/36/0/36     0.01        175000      idle
cmpgnode02    0/32/0/32     0.01        175000      idle
cmpgnode03    0/20/0/20     0.01        145000      idle
cmpgnode04    0/20/0/20     0.01        145000      idle
cmpgnode05    0/36/0/36     0.01        210000      idle
cmpgnode06    0/12/0/12     0.01        32768       idle
cmpgnode07    0/12/0/12     0.01        32768       idle
[root@binfservms01 ~]#
```

node
as03
as06
as07
as11
as15
as19
as27
as31

```
[root@binfservms01 ~]# clusterstate.sh
NODELIST          CPUS(A/I/O/T)    CPU_LOAD    FREEMEMORY      STATE
binfservas03      20/60/0/80     20.06       1844352        mixed
binfservas06      2/30/0/32      0.07        45200         mixed
binfservas07      16/0/0/16      2.30        242832        allocated
binfservas08      16/0/0/16      5.87        162960        allocated
binfservas09      16/0/0/16      2.73        242832        allocated
binfservas10      16/0/0/16      1.51        242832        allocated
binfservas11      16/8/0/24      1.79        242832        mixed
binfservas12      24/0/0/24      2.82        46224         allocated
binfservas13      16/8/0/24      1.70        242832        mixed
binfservas14      19/5/0/24      24.17       41104         mixed
binfservas15      17/11/0/28     1.84        230544        mixed
binfservas16      24/4/0/28      80.95       111760        mixed
binfservas17      16/12/0/28     2.51        242832        mixed
binfservas18      0/28/0/28      0.43        112385        idle
binfservas19      33/7/0/40      4.60        335184        mixed
binfservas20      33/7/0/40      4.45        335184        mixed
binfservas21      32/8/0/40      3.02        355664        mixed
binfservas22      32/8/0/40      2.96        355664        mixed
binfservas23      32/8/0/40      3.54        355664        mixed
binfservas24      32/8/0/40      3.34        355664        mixed
binfservas25      32/8/0/40      3.83        355664        mixed
binfservas26      32/8/0/40      4.26        355664        mixed
binfservas27      0/0/128/128    0.01        512000        down*
binfservas28      128/0/0/128    5.57        401664        allocated
binfservas29      128/0/0/128    4.76        376832        allocated
binfservas30      120/8/0/128    0.01        20480         mixed
```

Data Storage

Used ~ 900 TB (75% of total capacity)

/home/*username*

/data/projects/p*nnn_abcd*

/data/users/*username*

/scratch

/tmp

File servers

/home 1 TB

ms01

fs07

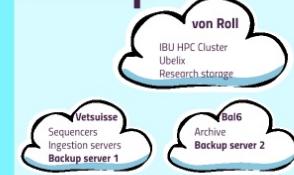
fs08

fs03

fs04

/data 1.3 PB

Backup



/scratch

/tmp

/scratch

/tmp

directories local to each node

/scratch

/tmp



directories local to each node

/scratch

/tmp



directories local to each node

during job execution: \$SCRATCH

/scratch

/tmp



directories local to each node

during job execution: \$SCRATCH

e.g. /scratch/172007

/scratch

/tmp



directories local to each node

during job execution: \$SCRATCH

e.g. /scratch/172007

deleted after job completion

/scratch

/tmp

directories local to each node

during job execution: \$SCRATCH

e.g. /scratch/172007

deleted after job completion

/scratch



directories local to each node
during job execution: \$SCRATCH
e.g. /scratch/172007
deleted after job completion

/tmp



quota (1GB)
use /scratch instead

Backup

von Roll

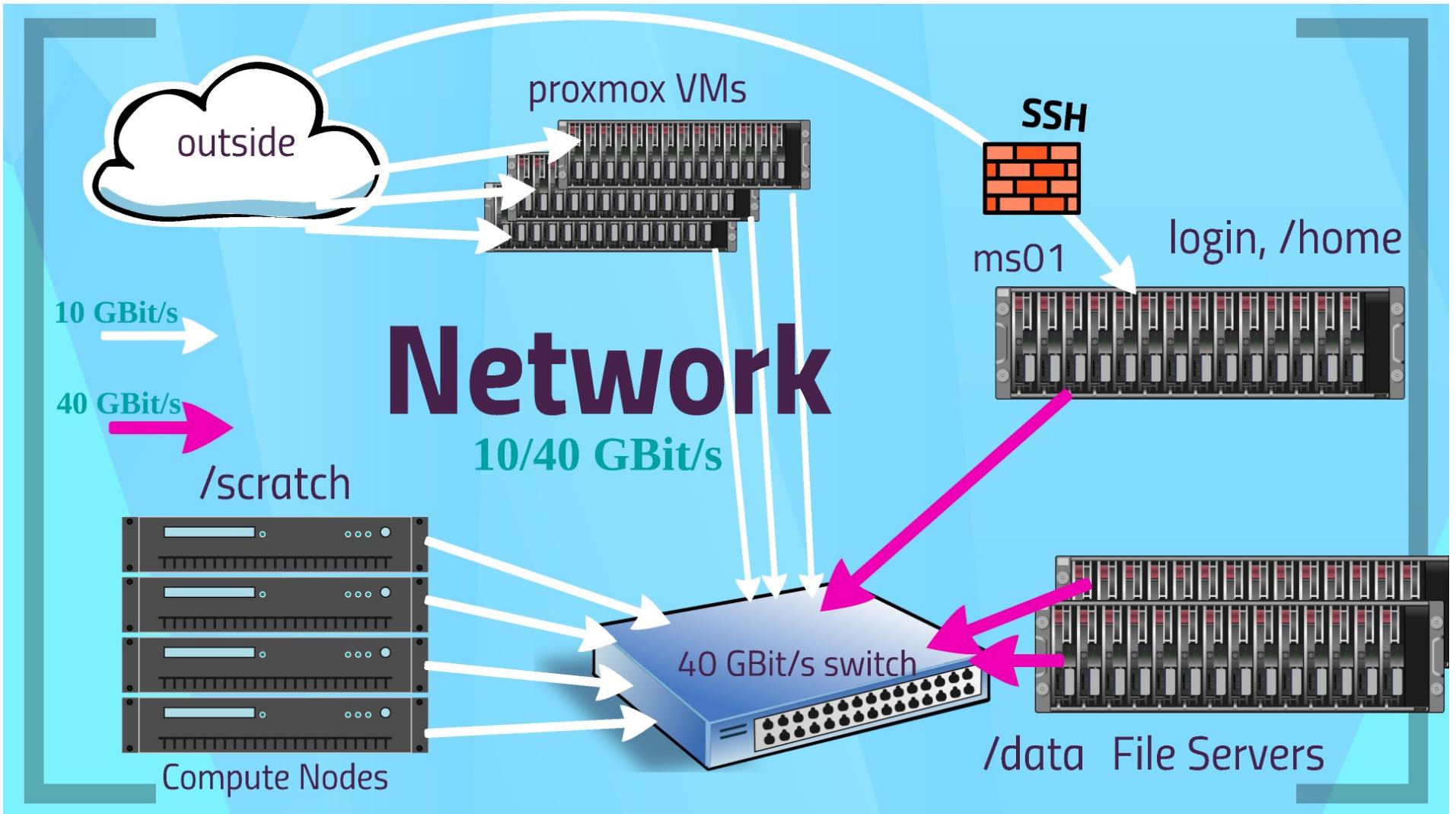
IBU HPC Cluster
Ubelix
Research storage

Vetsuisse

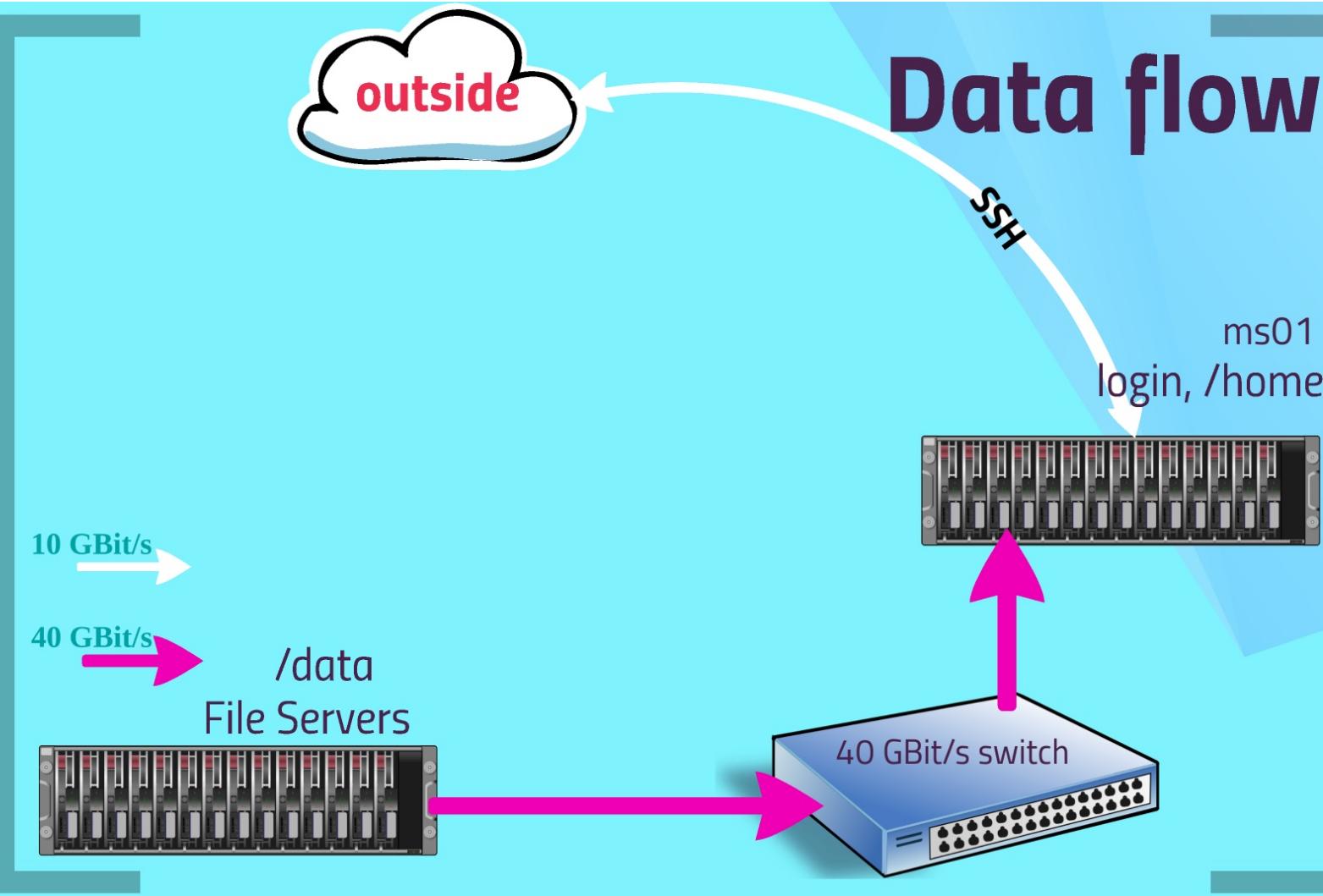
Sequencers
Ingestion servers
Backup server 1

Bal6

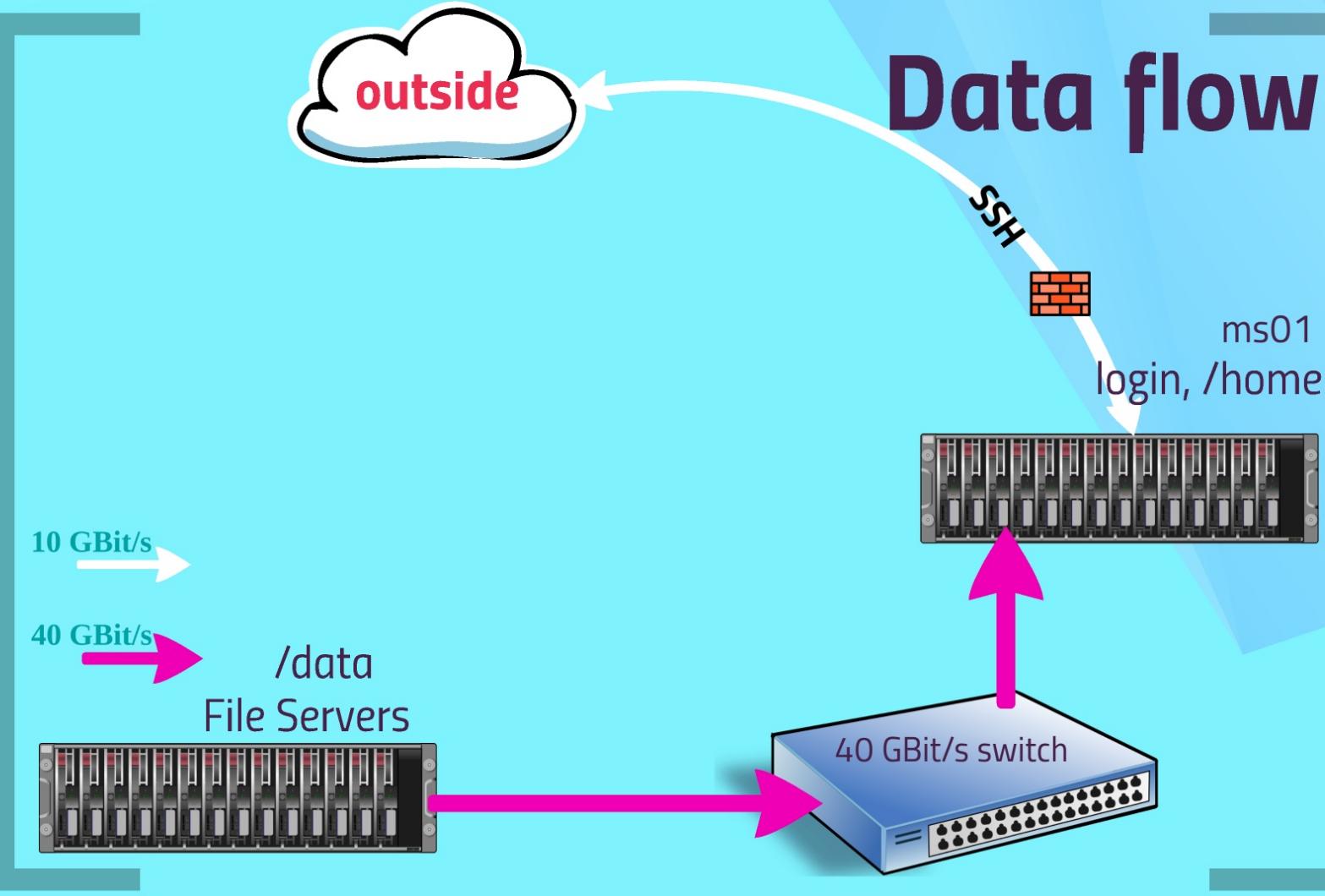
Archive
Backup server 2



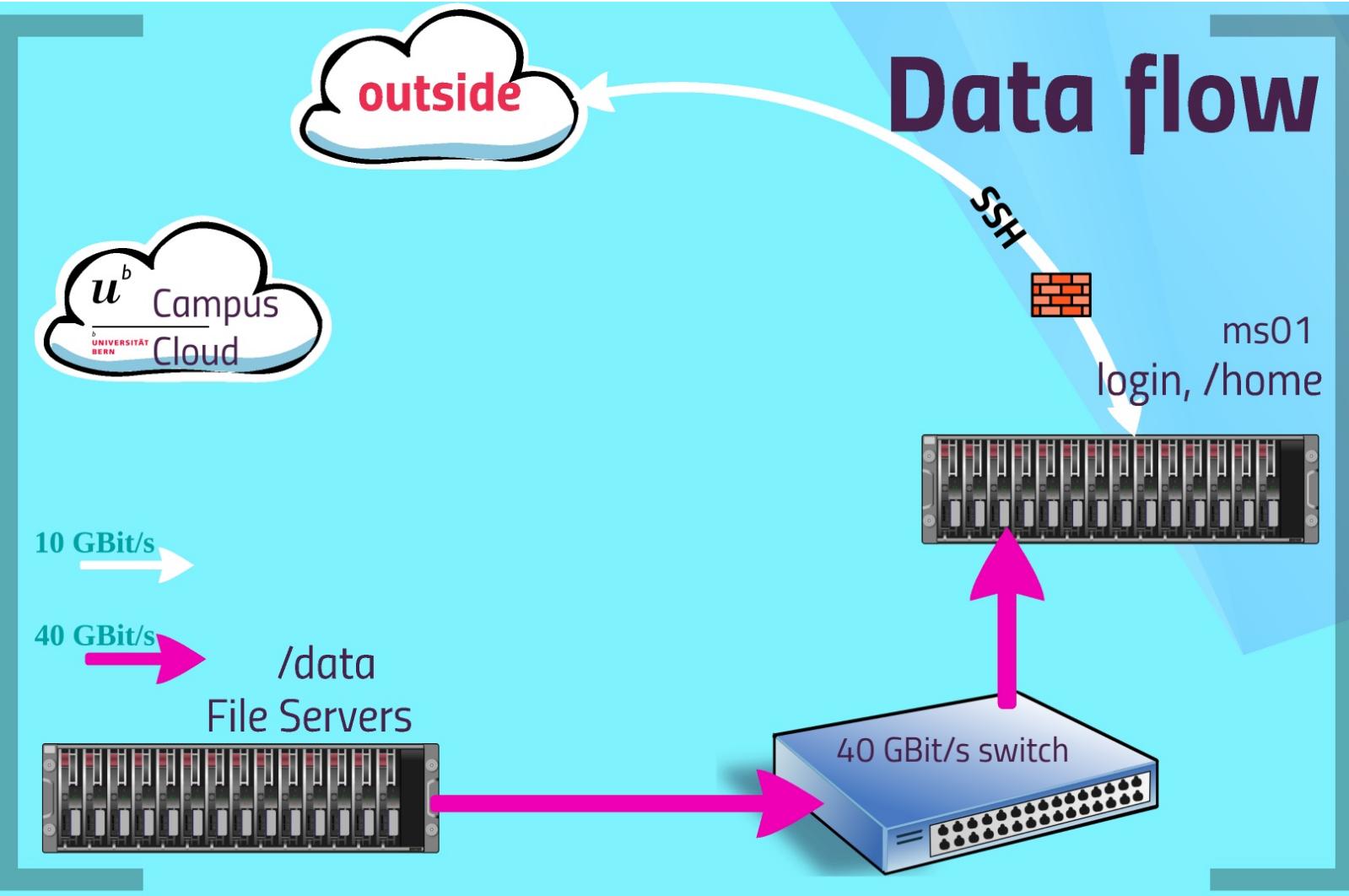
Data flow



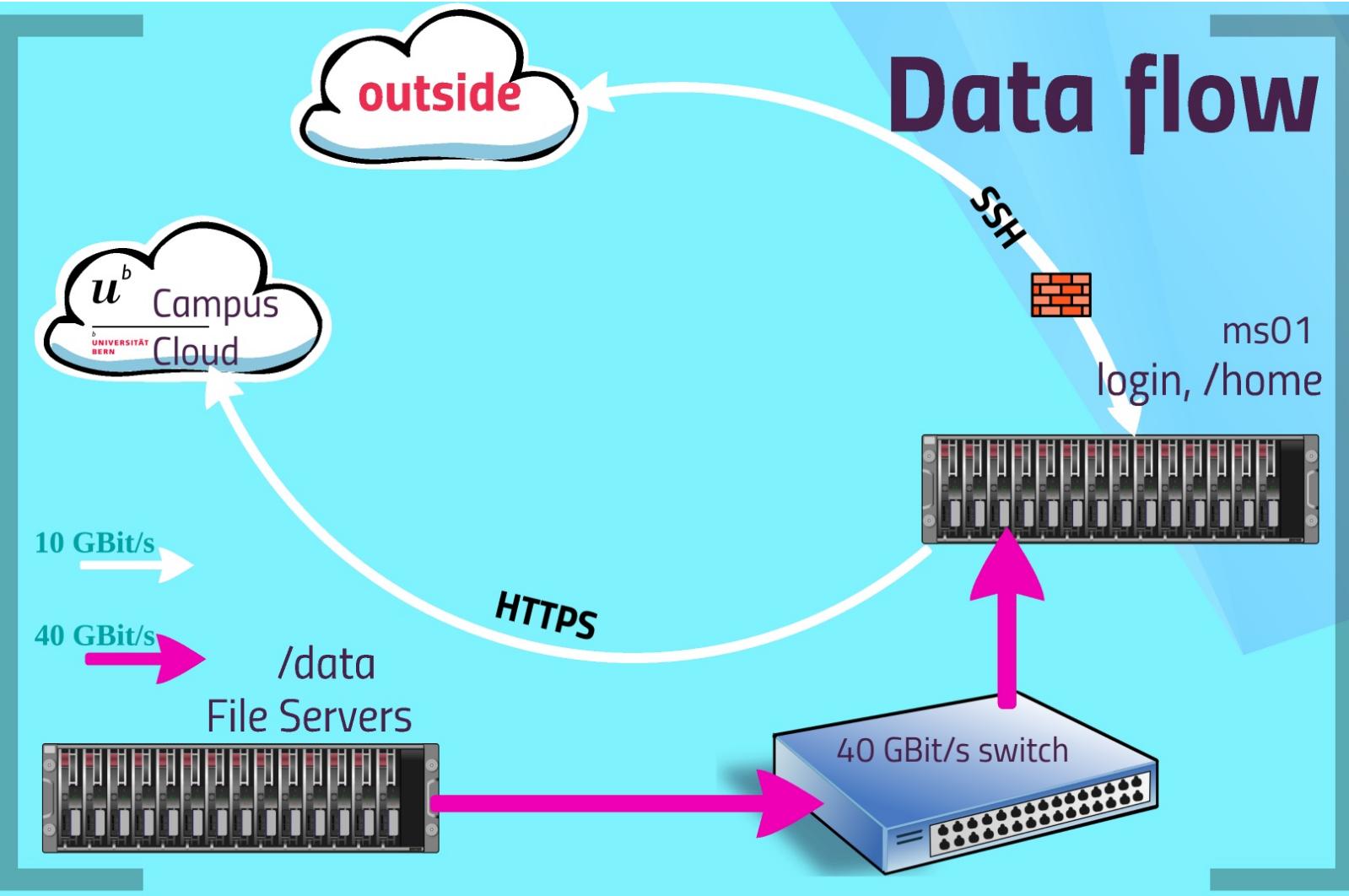
Data flow



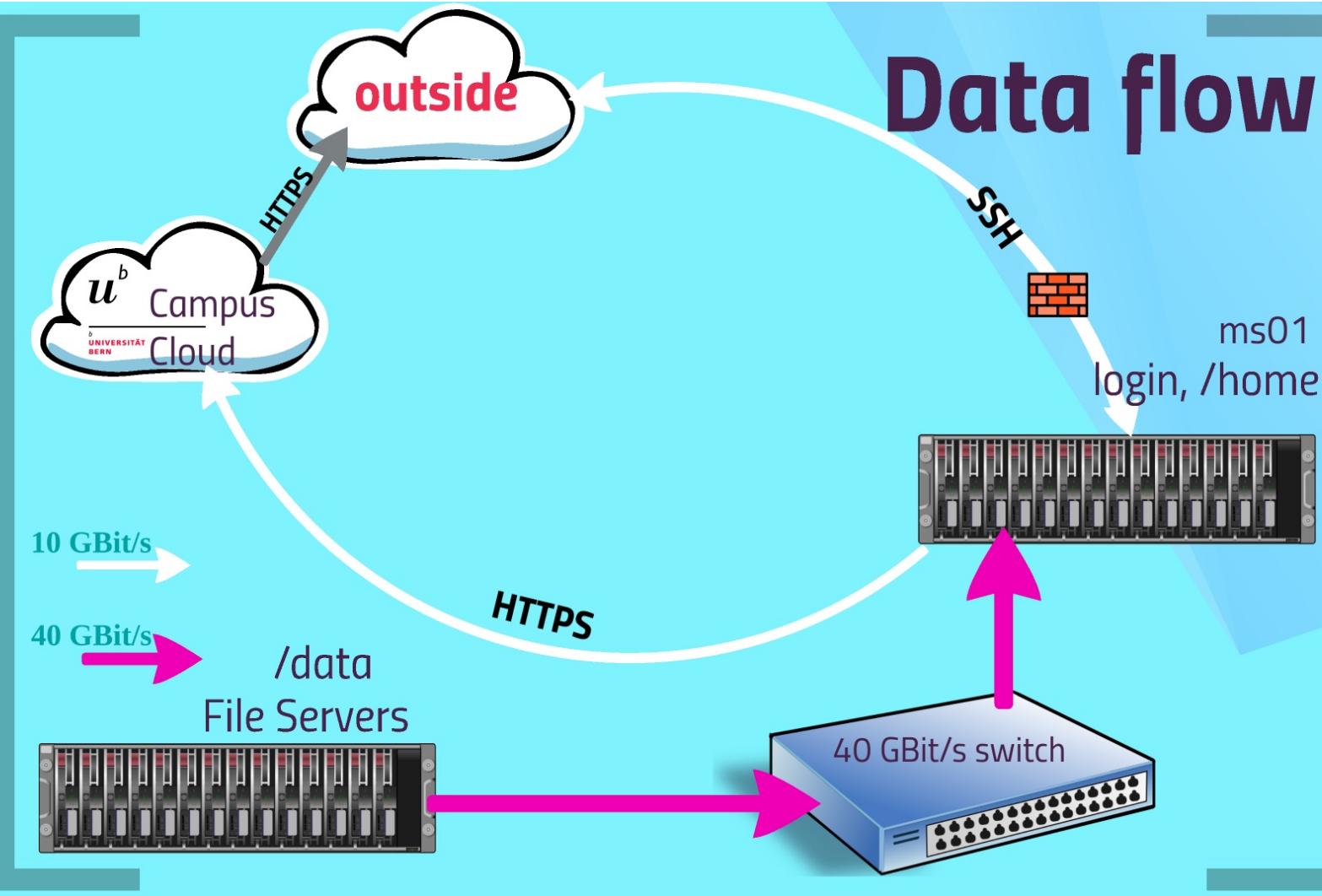
Data flow



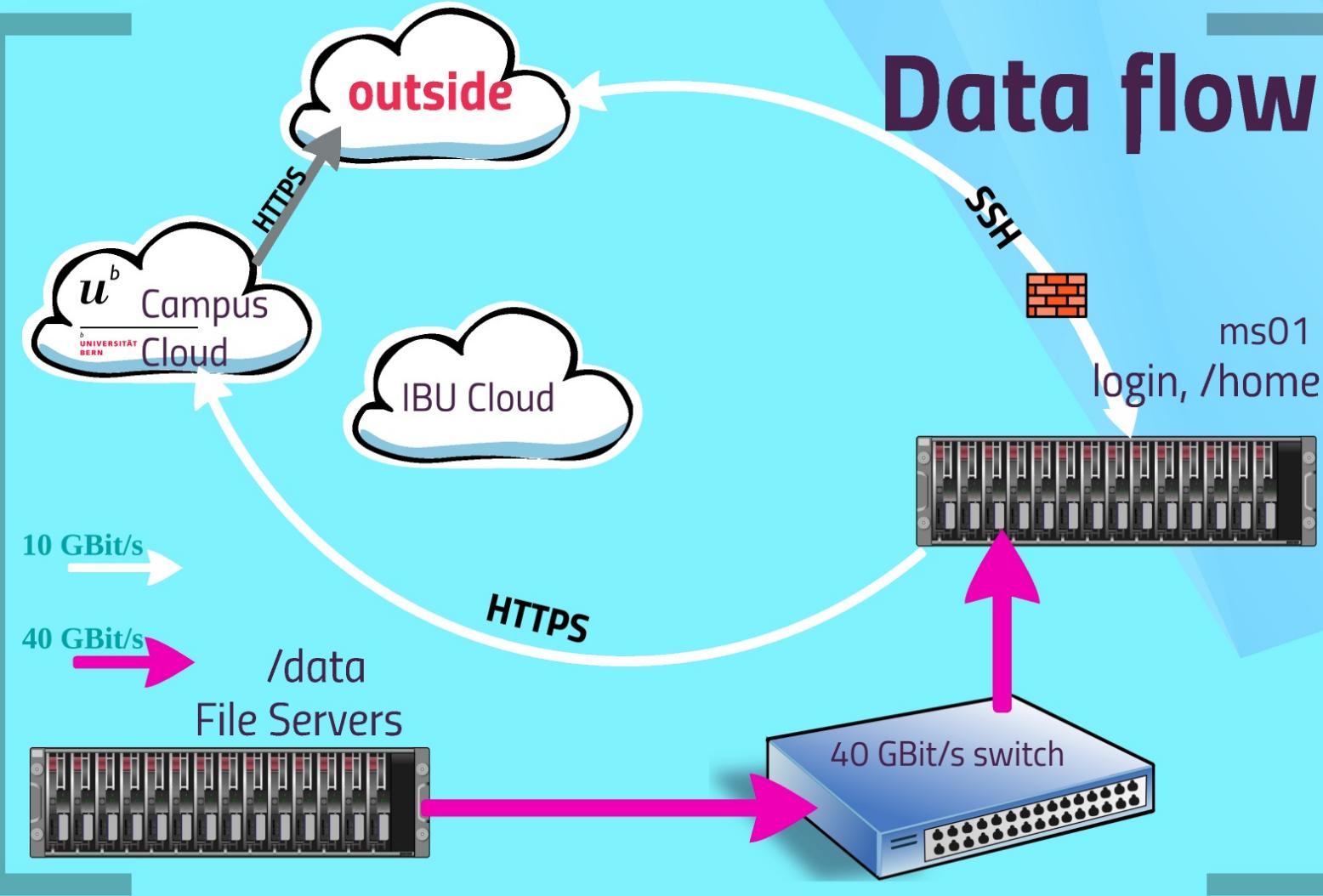
Data flow



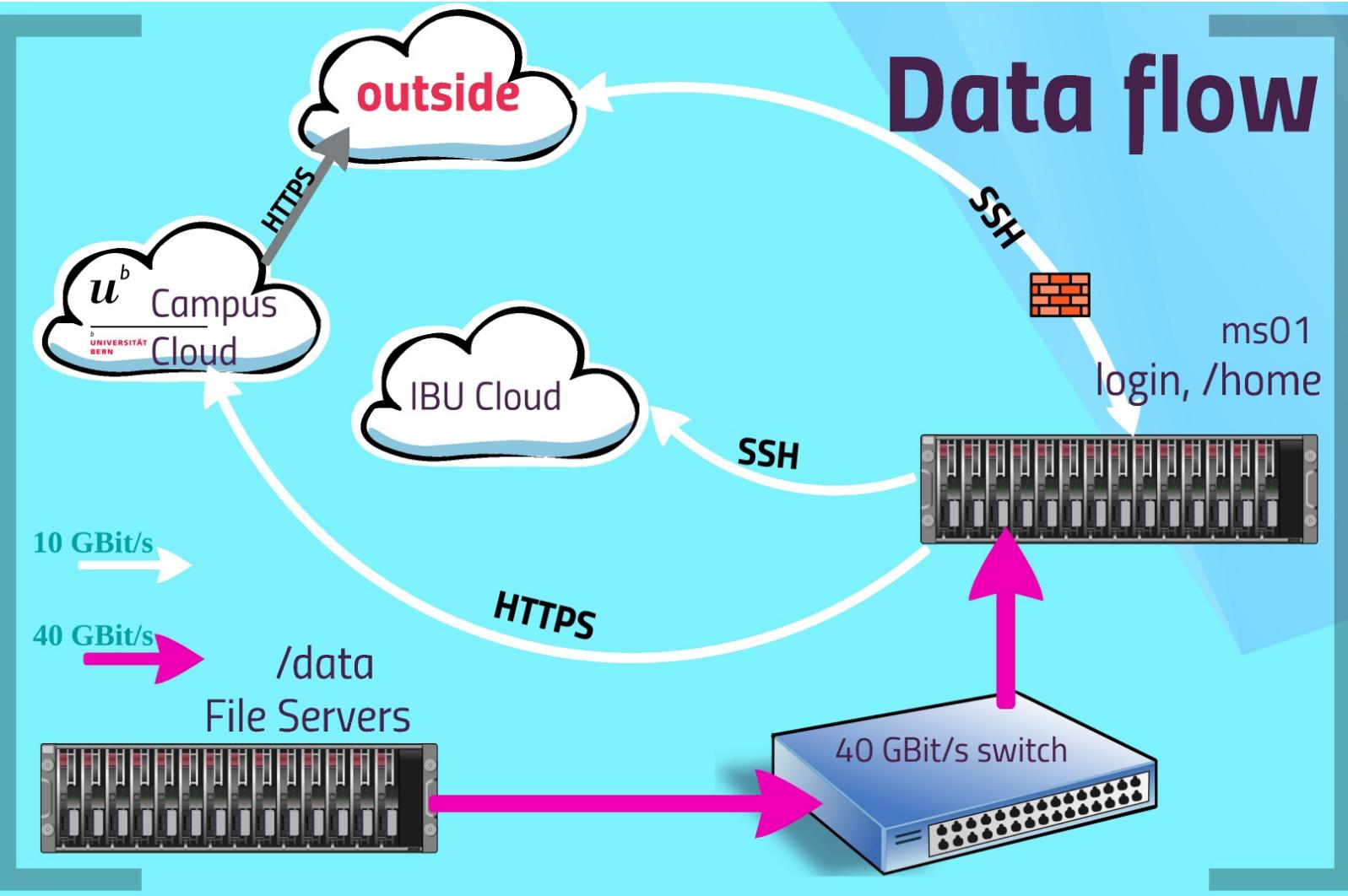
Data flow



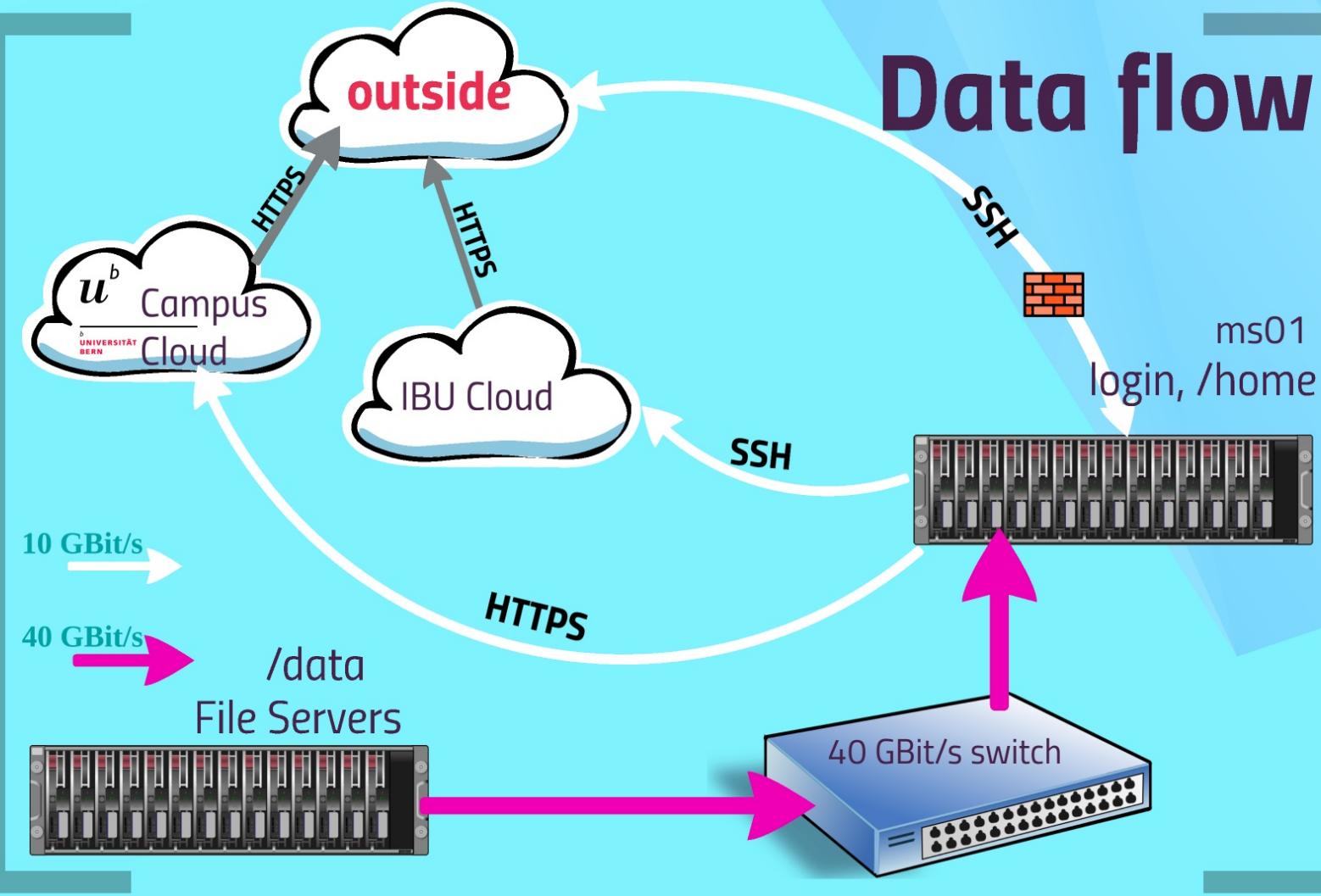
Data flow



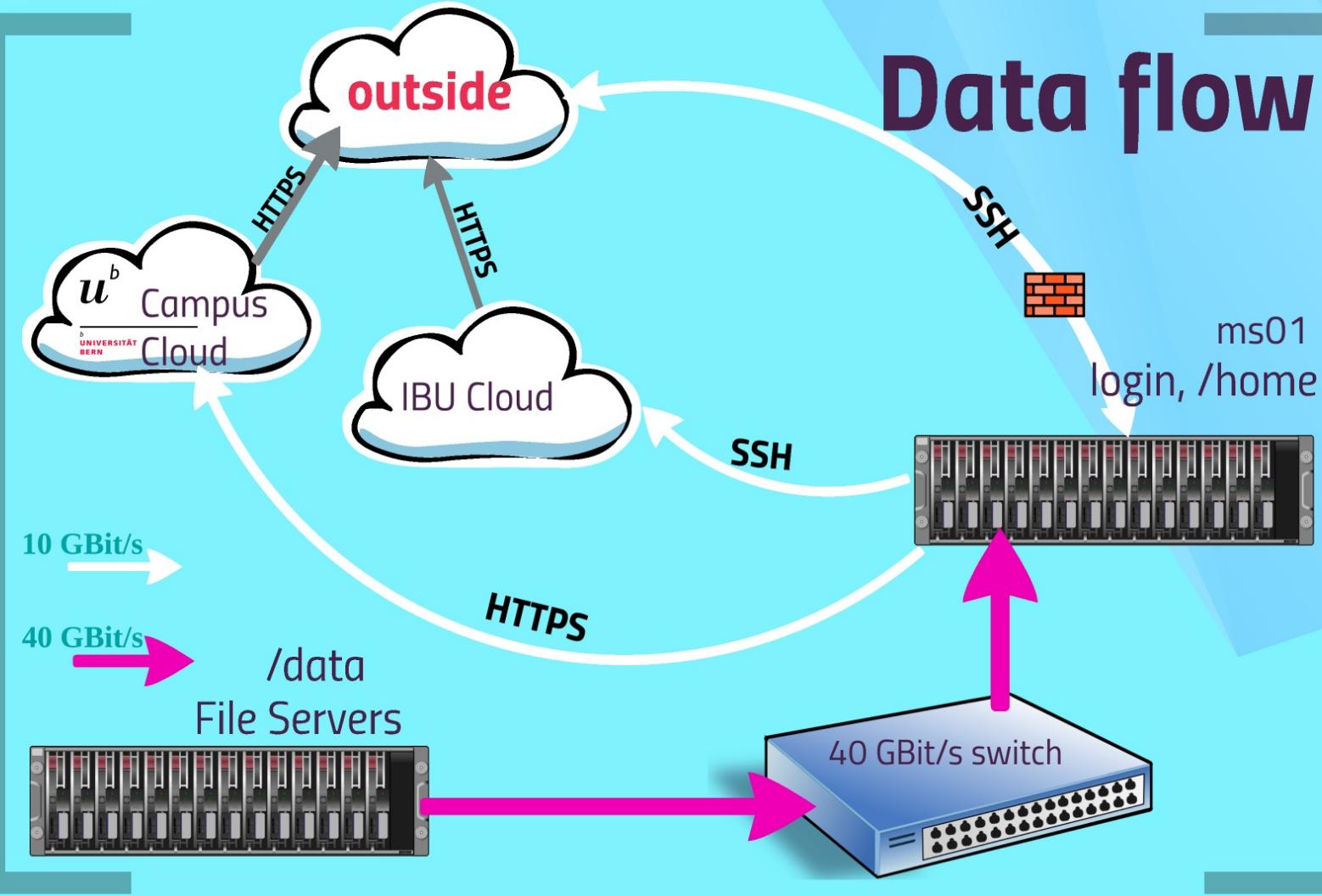
Data flow



Data flow



Data flow



Take home



do not start computation on head node, use an interactive job

use /scratch whenever possible, do not use /tmp

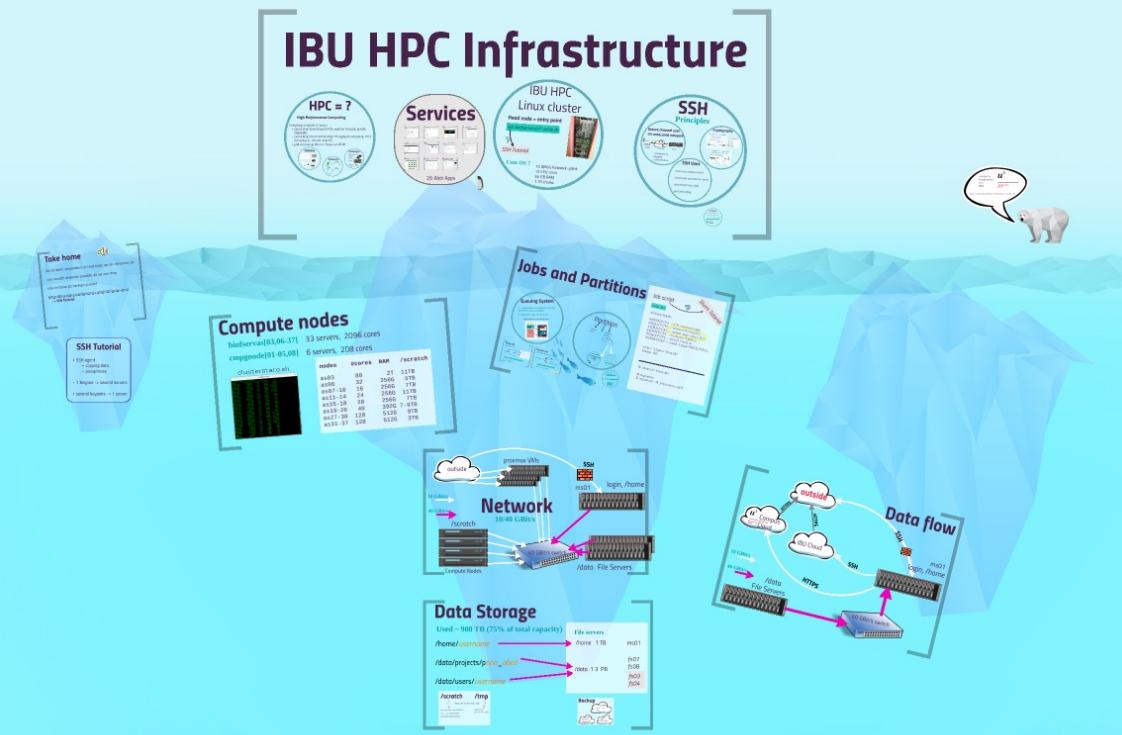
take initiative for backups yourself

<https://docs.pages.bioinformatics.unibe.ch/cluster-docs/>

-> SSH Tutorial

SSH Tutorial

- SSH agent
 - copying data
 - passphrase
- 1 Keypair -> several servers
- several keypairs -> 1 server



Interfaculty Bioinformatics Unit

Pierre Berthier, University of Bern, 31.10.2022