Machine & Deep Learning Tutorial

USING HIGH PERFORMANCE COMPUTING

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PRACTICAL LECTURE 1

Short Introduction to UNIX & SSH

December 05, 2019
In-Telegence, ON4OFF Training

ON 4 OFF

UNIVERSITY OF ICELAND
SCHOOL OF ENGINEERING AND NATURAL SCIENCES
FACULTY OF INDUSTRIAL ENGINEERING, MECHANICAL ENGINEERING AND COMPUTER SCIENCE

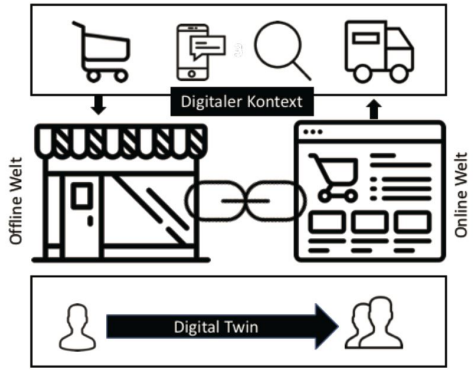
JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

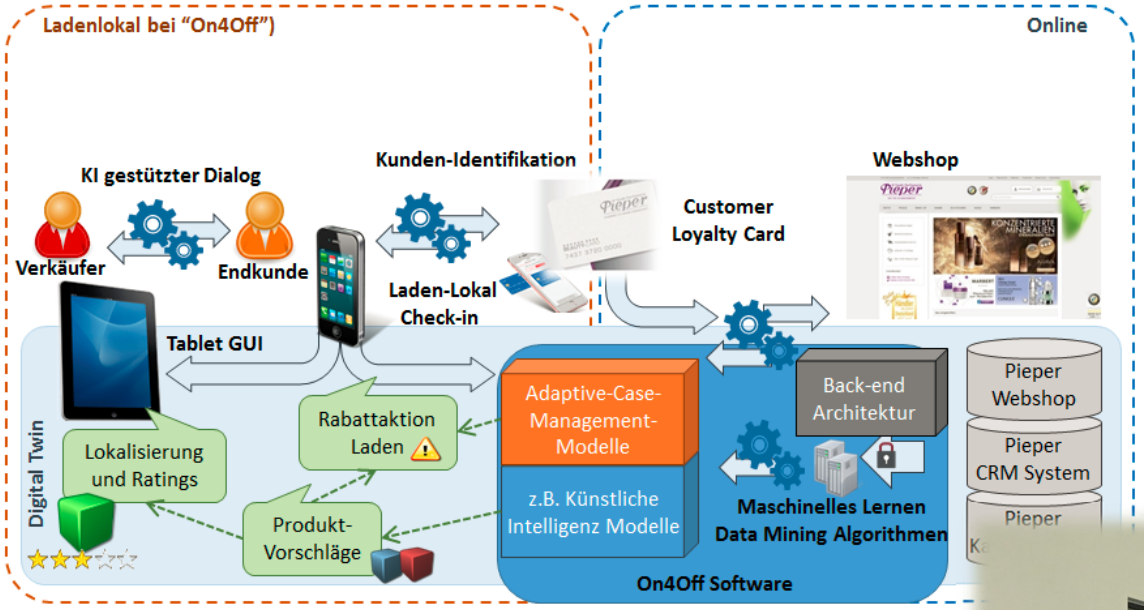
DEEP Projects

HELMHOLTZ AI | ARTIFICIAL INTELLIGENCE COOPERATION UNIT

ON4OFF Project in Context

- Retail Examples





[6] ON4OFF Web page

Using Machine & Deep Learning to enable better online-offline shopping in Germany

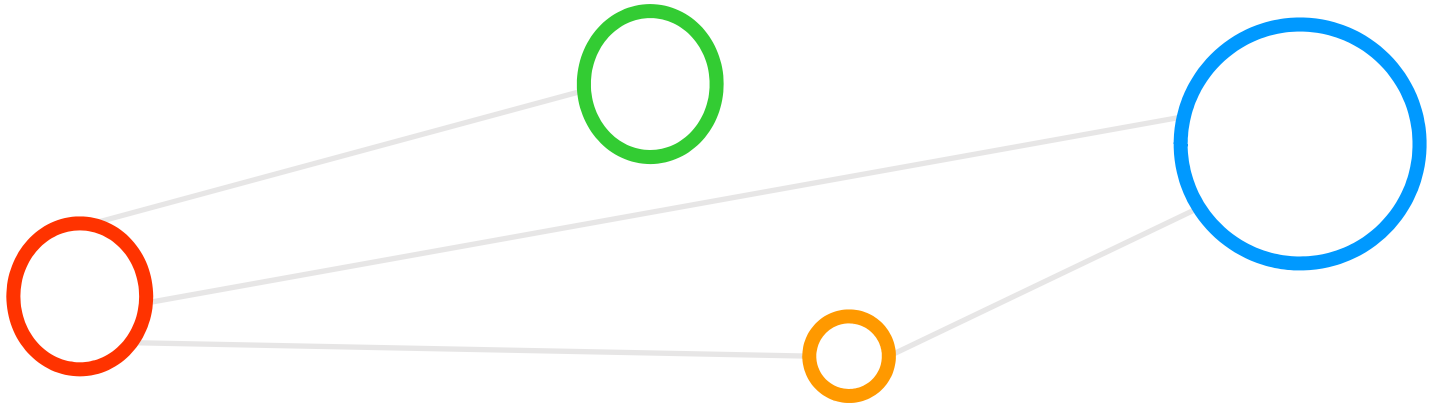
Outline

- Using UNIX on HPC Systems
  - HPC Systems & Modular Supercomputing Architecture
  - HPC System Examples DEEP & Jötunn
  - Selected UNIX Commands
  - Module Environment
  - Basic Editor VI

- Using SSH to connect to HPC Systems
  - SSH Clients
  - Private/Public Key Pairs
  - SSH Key Example Login HPC System DEEP
  - Username & Password Example HPC System Jötunn
  - Workaround for external login to HPC System Jötunn

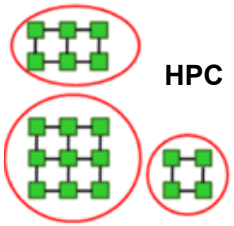
- **This lecture is not considered to be a full introduction to UNIX and SSH and rather focusses on selected commands and concepts relevant for assignments**
- **The goal of this lecture is to make course participants aware of the UNIX environments existing on world-wide HPC systems and how to connect to them using the SSH protocol**

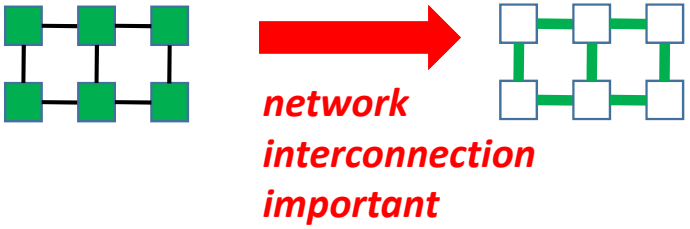
Using UNIX on HPC Systems



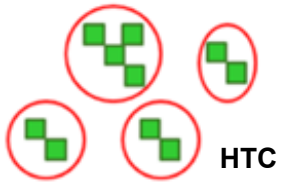
Understanding HPC Systems

- **High Performance Computing (HPC) is based on computing resources that enable the efficient use of parallel computing techniques through specific support with dedicated hardware such as high performance cpu/core interconnections.**





- **High Throughput Computing (HTC) is based on commonly available computing resources such as commodity PCs and small clusters that enable the execution of 'farming jobs' without providing a high performance interconnection between the cpu/cores.**



HPC & Data-intensive Sciences – A Field of Constant Evolution

1.000.000 FLOP/s

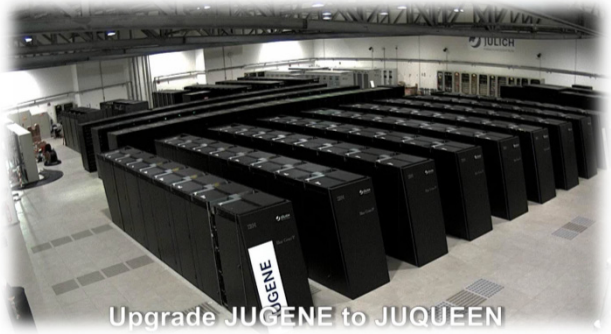
~1984

© Photograph by Rama, Wikimedia Commons

- **Floating Point Operations per one second (FLOPS or FLOP/s)**
- **1 GigaFlop/s = 10^9 FLOPS**
- **1 TeraFlop/s = 10^{12} FLOPS**
- **1 PetaFlop/s = 10^{15} FLOPS**
- **1 ExaFlop/s = 10^{18} FLOPS**

1.000.000.000.000.000 FLOP/s

~295.000 cores~2009 (JUGENE)



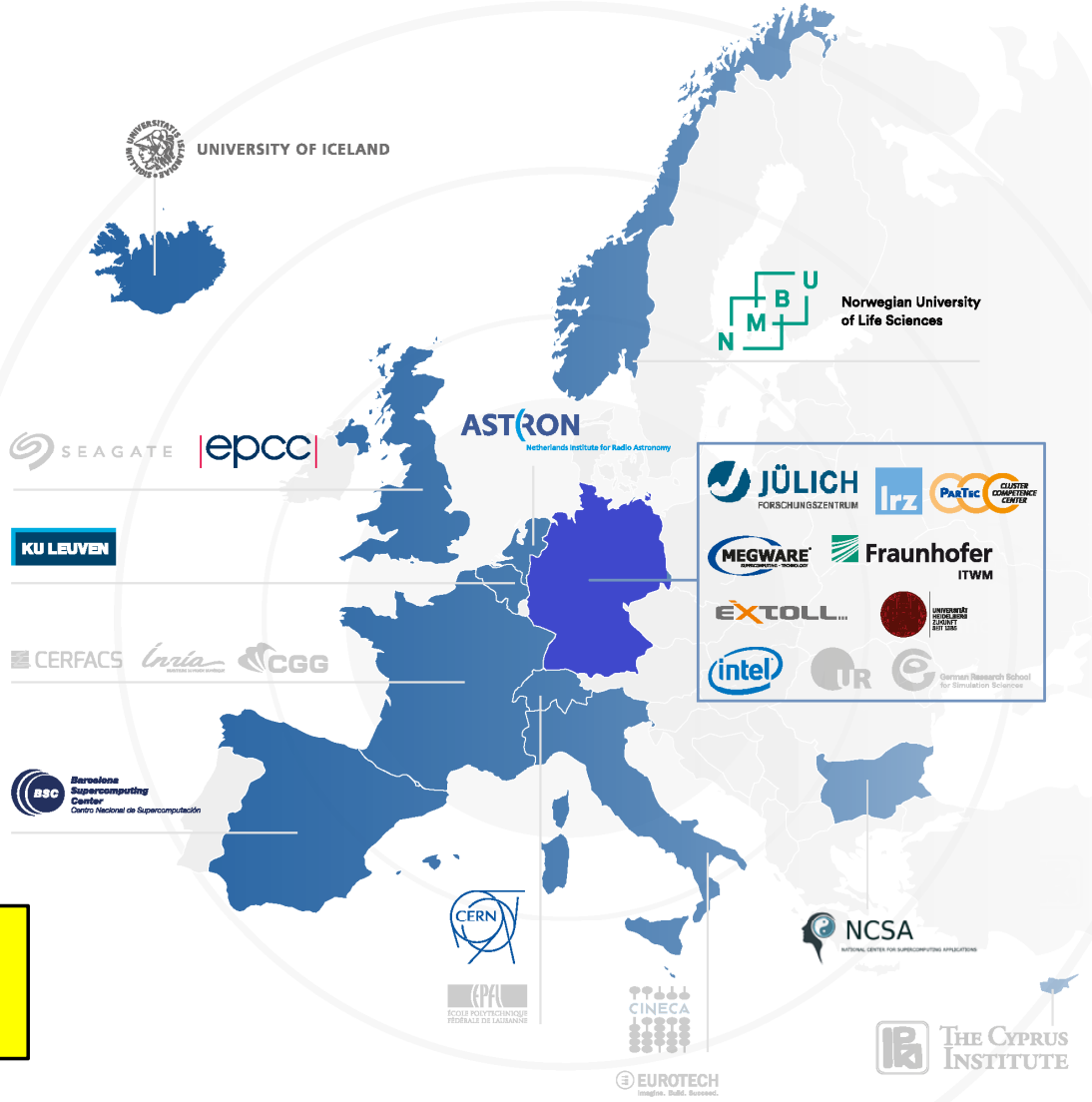
>5.900.000.000.000.000 FLOP/s
~ 500.000 cores
~2013 → end of service in 2018

DEEP series of PROJECTS & HPC

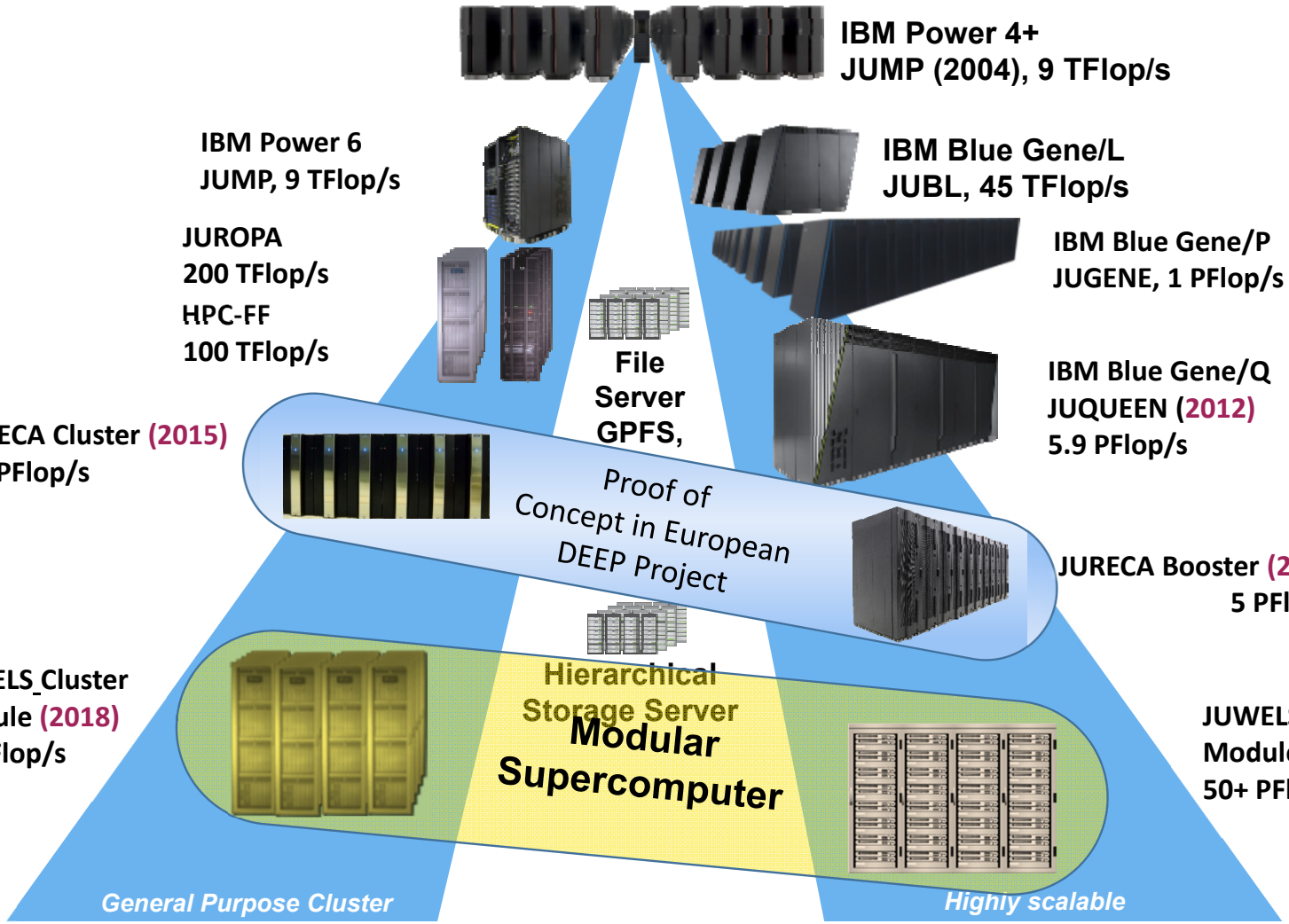
- 3 EU Exascale projects
  DEEP, DEEP-ER, DEEP-EST
- 27 partners
  Coordinated by JSC
- EU-funding: 30 M€
  JSC-part > 5,3 M€
- Nov 2011 – Dec 2020

- **Strong collaboration with our industry partners Intel, Extoll & Megware**

- **Juelich Supercomputing Centre implements the DEEP projects designs in its HPC production infrastructure**

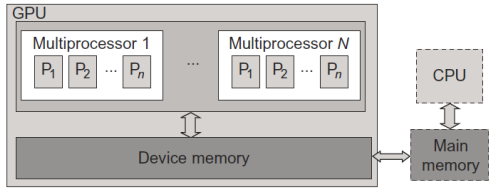


[3] DEEP Projects Web Page


IBM Power 4+
JUMP (2004), 9 TFlop/s
IBM Power 6
JUMP, 9 TFlop/s
IBM Blue Gene/L
JUBL, 45 TFlop/s
JUROPA
200 TFlop/s
HPC-FF
100 TFlop/s
IBM Blue Gene/P
JUGENE, 1 PFlop/s
File
Server
GPFS,
IBM Blue Gene/Q
JUQUEEN (2012)
5.9 PFlop/s
JURECA Cluster (2015)
2.2 PFlop/s
Proof of
Concept in European
DEEP Project
JURECA Booster (2017)
5 PFlop/s
Hierarchical
Storage Server
JUWELS Cluster
Module (2018)
12 PFlop/s
Modular
Supercomputer
JUWELS Scalable
Module (2019/20)
50+ PFlop/s
General Purpose Cluster
Highly scalable

HPC System – DEEP Testcluster

- DEEP-EST Project Prototype HPC System
  - Dynamical Exascale Entry Platform (DEEP)
- Implements Modular Supercomputing Architecture (MSA)
  - Cluster module (installed at JSC in April 2019)
  - Extreme Scale Booster module (to be installed during 2019)
  - Data Analytics module (to be installed during 2019, prototype available)
- Data Analytics Module (DAM) prototype
  - 3 nodes x 4 Graphics Processing Units (GPUs)
  - Each node with 4 x Nvidia Tesla V100 GPU
  - Each node with host CPUs:
    2 x Intel Xeon 'Skylake' Silver 4112
  - Access via common DEEP environment



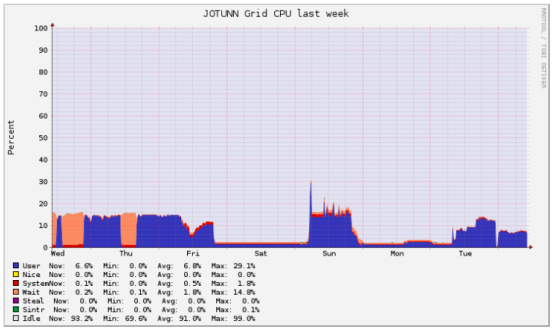
[4] Distributed & Cloud Computing Book

[2] DEEP Test Cluster

➢ **We will use the modular supercomputing architecture on the DEEP test cluster with deep learning and Graphic Processing Units (GPUs)**

HPC System – Jötunn Cluster Example

- 4 Nodes
  - Cpu: 2x Intel Xeon CPU E5-2690 v3 @ 2.60GHz (2.6 GHz, 12 core)
- Memory
  - 128GB DDR4
- Interconnect
  - 10 Gb/s Ethernet
- Ganglia monitoring service
  - Shows usage of CPUs



[1] Icelandic HPC Machines & Community

Selected UNIX Commands: hostname

- Example: ‘hostname -A’ command on our Jötunn cluster

```
[morris@jotunn ~]$ hostname -A
jotunn-login2.rhi.hi.is jotunn jotunn.rhi.hi.is
[morris@jotunn ~]$ exit
logout
Connection to jotunn.rhi.hi.is closed.
```

[1] Icelandic HPC Machines & Community

- Example: ‘hostname -A’ command on our DEEP Testcluster

```
[riedel1@deepv ~]$ hostname -A
deepv.deep zam1015.zam.kfa-juelich.de deepvm.deep
```

[2] DEEP Test Cluster

Selected UNIX Commands: whoami & clear

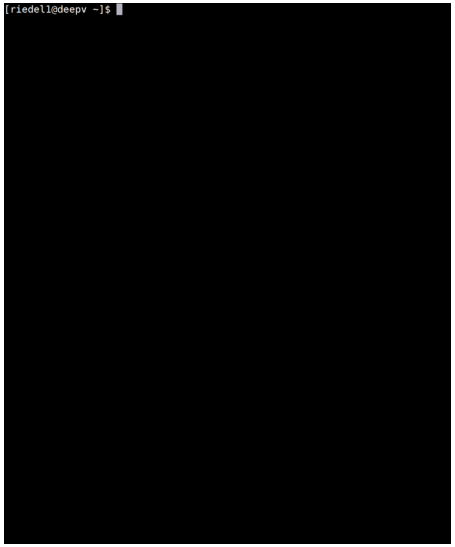
- Example: ‘whoami’ command on our DEEP Testcluster

```
[riedel1@deepv ~]$ whoami
riedel1
```

[1] Icelandic HPC Machines & Community

- Example: ‘clear’ command on our DEEP Testcluster

```
Last login: Thu Aug 29 08:20:33 2019 from pd95b302c.dip0.t-ipconnect.de
################################################################
#                                                              #
#                          DEEP Testcluster                    #
#                                                              #
################################################################
#                                                              #
# Useful job status tools:                                     #
#                                                              #
# Overall node usage: slurmtop                                 #
# Show jobs in the system: squeue                              #
# List reservations: scontrol show res                         #
# Check job issues: scontrol show job <jobid>                  #
# See /etc/slurm/README for details and known problems         #
#                                                              #
################################################################
#                                                              #
# /usr/local now served by local beegfs file system.           #
# performance issues under investigation.                      #
# pn Thu Jun 13 14:26:48 CEST 2019                             #
#                                                              #
################################################################
#                                                              #
# The transition to the new software stack will happen on Tuesday 9th #
# To enable it now use "enable_new_software_stack"             #
# To enable the current stack use "enable_old_stack"           #
# To enable the legacy stack use "enable_legacy_stack"         #
#                                                              #
################################################################
#                                                              #
# /usr/local on deepv, dp-cn nodes:                            #
# now mounted without acls and extended attributes.            #
# cm/pn Fri Jul 26 10:30:50 CEST 2019                          #
#                                                              #
################################################################
[riedel1@deepv ~]$ whoami
riedel1
[riedel1@deepv ~]$ hostname -f
deepv.deep
[riedel1@deepv ~]$ hostname -A
deepv.deep zam1015.zam.kfa-juelich.de deepvm.deep
[riedel1@deepv ~]$ clear
```



Selected UNIX Commands: ls & pwd

- Example: ‘ls -al’ command on our DEEP Testcluster

```
[riedel1@deepv ~]$ ls -al
total 14
drwx------ 10 riedel1 jusers 4096 Aug 29 08:20 .
drwxr-xr-x  8 root    root   4096 May 14 17:03 ..
-rw-------  1 riedel1 jusers 2613 Aug 16 17:40 .bash_history
-rwx------  1 riedel1 jusers  535 Nov 30  2018 .bash_profile
-rwx------  1 riedel1 jusers  501 Nov 30  2018 .bashrc
drwx------  6 riedel1 jusers 4096 Aug 15 13:30 .cache
drwxr-xr-x  3 riedel1 jusers 4096 Aug 15 13:30 .config
drwxr-xr-x  6 riedel1 jusers 4096 Aug 15 19:51 hugi
drwxr-xr-x  2 riedel1 jusers 4096 Aug 15 13:30 .keras
drwxr-xr-x  3 riedel1 jusers 4096 Aug 15 11:54 .lmod.d
drwx------  4 riedel1 jusers 4096 Aug 15 13:20 .local
drwxr-xr-x  5 riedel1 jusers 4096 Aug 15 14:00 project
lrwxrwxrwx  1 riedel1 jusers    9 Nov 30  2018 shared -> ../shared
drwx------  2 riedel1 jusers 4096 Nov 30  2018 .ssh
-rw-------  1 riedel1 jusers 2530 Aug 15 14:00 .viminfo
-rw-------  1 riedel1 jusers  204 Aug 29 08:20 .Xauthority
```

- Example: ‘pwd’ command on our DEEP Testcluster

```
[riedel1@deepv ~]$ cd HPC-Course-Fall-2019/
[riedel1@deepv HPC-Course-Fall-2019]$ pwd
/p/home/jusers/riedel1/deep/HPC-Course-Fall-2019
```

[2] DEEP Test Cluster

Selected UNIX Commands: mkdir & cd

- Example: ‘mkdir FOLDER’ and ‘cd FOLDER’ command on our DEEP Testcluster

```
[riedel1@deepv ~]$ mkdir HPC-Course-Fall-2019
[riedel1@deepv ~]$ ls -al
total 15
drwx------ 11 riedel1 jusers 4096 Aug 29 09:30 .
drwxr-xr-x  8 root    root   4096 May 14 17:03 ..
-rw-------  1 riedel1 jusers 2713 Aug 29 09:30 .bash_history
-rwx------  1 riedel1 jusers  535 Nov 30  2018 .bash_profile
-rwx------  1 riedel1 jusers  501 Nov 30  2018 .bashrc
drwx------  6 riedel1 jusers 4096 Aug 15 13:30 .cache
drwxr-xr-x  3 riedel1 jusers 4096 Aug 15 13:30 .config
drwxr-xr-x  2 riedel1 jusers 4096 Aug 29 09:30 HPC-Course-Fall-2019
drwxr-xr-x  6 riedel1 jusers 4096 Aug 15 19:51 hugi
drwxr-xr-x  2 riedel1 jusers 4096 Aug 15 13:30 .keras
drwxr-xr-x  3 riedel1 jusers 4096 Aug 15 11:54 .lmod.d
drwx------  4 riedel1 jusers 4096 Aug 15 13:20 .local
drwxr-xr-x  5 riedel1 jusers 4096 Aug 15 14:00 project
lrwxrwxrwx  1 riedel1 jusers    9 Nov 30  2018 shared -> ../shared
drwx------  2 riedel1 jusers 4096 Aug 29 09:28 .ssh
-rw-------  1 riedel1 jusers 2530 Aug 15 14:00 .viminfo
-rw-------  1 riedel1 jusers  204 Aug 29 09:30 .Xauthority
[riedel1@deepv ~]$ cd HPC-Course-Fall-2019
[riedel1@deepv HPC-Course-Fall-2019]$ ls -al
total 2
drwxr-xr-x  2 riedel1 jusers 4096 Aug 29 09:30 .
drwx------ 11 riedel1 jusers 4096 Aug 29 09:30 ..
```

[2] DEEP Test Cluster

HPC System Module Environment

- Knowledge of installed compilers essential (e.g. C, Fortran90, etc.)
  - Different versions and types of compilers exist (Intel, GNU, MPI, etc.)
  - E.g. mpicc pingpong.c –o pingpong
- Module environment tool
  - Avoids to manually setup environment information for every application
  - Simplifies shell initialization and lets users easily modify their environment
  - Modules can be loaded and unloaded
  - Enable the installation of software in different versions
- Module avail
  - Lists all available modules on the HPC system (e.g. compilers, MPI, etc.)
- Module load
  - Loads particular modules into the current work environment
  - E.g. module load gnu openmpi

[2] DEEP Test Cluster

HPC System Module Environment: module avail & module load

- Example: ‘module avail’ & ‘module load’ command on our DEEP Testcluster

```
[riedel1@deepv ~]$ module avail

---------- /usr/local/software/skylake/Stages/2019a/modules/all/Compiler/GCCcore/8.3.0 ----------
   Autotools/20180311                      PAPI/5.7.0
   Bazel/0.20.0                            Perl/5.28.1
   CMake/3.14.0                            PostgreSQL/11.2
   Clang/8.0.0-GCC-8.3.0-CUDA-10.1.105 (g)    Python/2.7.16
   CubeGUI/4.4.3                           Python/3.6.8                    (D)
   CubeLib/4.4.3                           SciPy-Stack/2019a-Python-2.7.16
   CubeWriter/4.4.2                        SciPy-Stack/2019a-Python-3.6.8  (D)
   Doxygen/1.8.15                          Tcl/8.6.9
   GEOS/3.7.1-Python-3.6.8                 TensorFlow/1.13.1-GPU-Python-3.6.8 (g)
   GMP/6.1.2                               UCX/1.5.1
   Graphviz/2.40.1                         X11/20190311
   HDF5/1.10.5-serial                      cURL/7.64.1
   LLVM/8.0.0                              flex/2.6.4
   Mesa/19.0.1                             h5py/2.9.0-serial-Python-3.6.8
   Meson/0.50.0-Python-3.6.8               numactl/2.0.12
   NCCL/2.4.6-1-CUDA-10.1.105          (g)    unzip/6.0
   Ninja/1.9.0

--------------------- /usr/local/software/skylake/Stages/2019a/UI/Compilers ---------------------
   GCC/8.3.0    Intel/2019.3.199-GCC-8.3.0

---------------------- /usr/local/software/skylake/Stages/2019a/UI/Tools ----------------------
   Advisor/2019_update3        Inspector/2019_update3    cuDNN/7.5.1.10-CUDA-10.1.105 (g)
   CUDA/10.1.105        (g)    JUBE/2.2.2                intel-para/2019a-mt
   EasyBuild/3.8.1             Java/1.8                  intel-para/2019a            (D)
   EasyBuild/3.9.1      (D)    VTune/2019_update3        tbb/2019.4.199

---------------------------------- /usr/local/software/extoll ----------------------------------
   extoll    openmpi/1.6.1_extoll

  Where:
   g:  built for GPU
   D:  Default Module

Use "module spider" to find all possible modules.
Use "module keyword key1 key2 ..." to search for all possible modules matching any of the "keys".
```

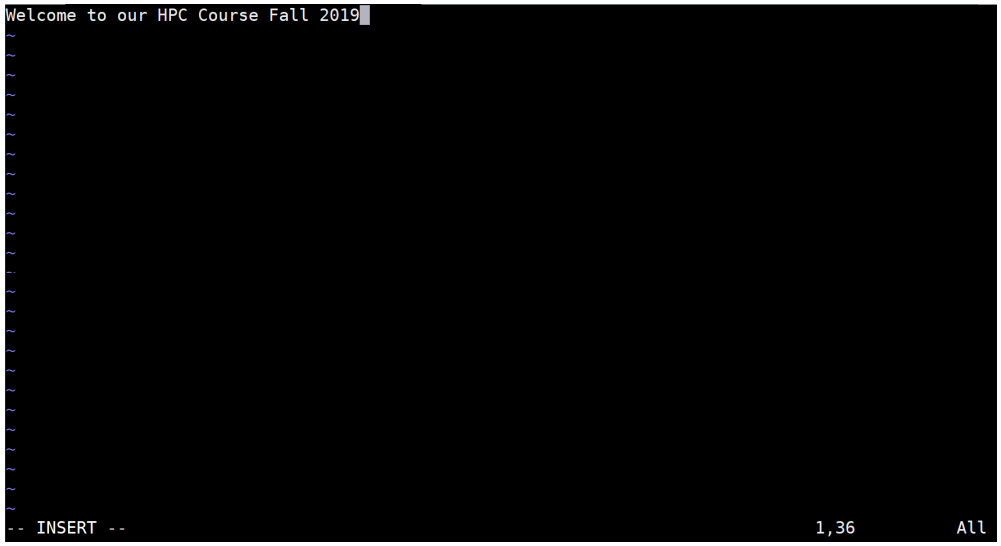
```
[riedel1@deepv HPC-Course-Fall-2019]$ module load Python/3.6.8
```

[2] DEEP Test Cluster

HPC System Environment Basic Editor VI

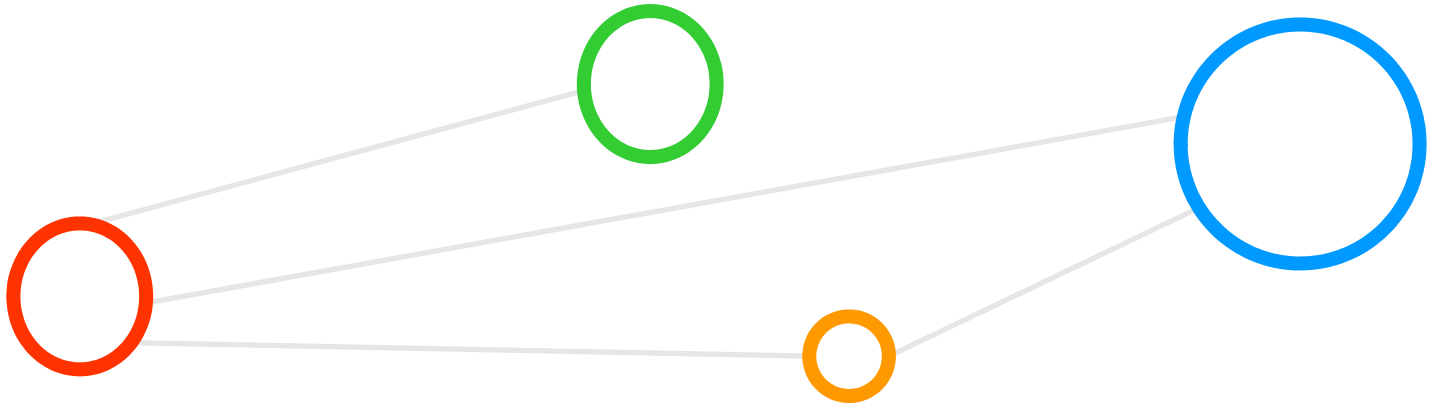
- HPC Systems have often not a GUI editor
  - Simple editor VI is always available
- Example: ‘vi FILENAME’ using command ‘:a’ to insert

```
[riedel1@deepv HPC-Course-Fall-2019]$ vi testfile
```



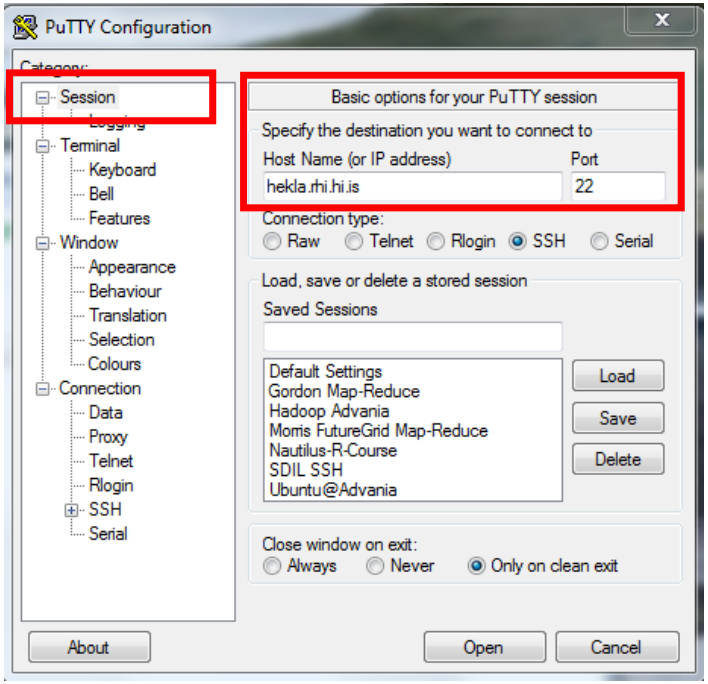
[2] DEEP Test Cluster

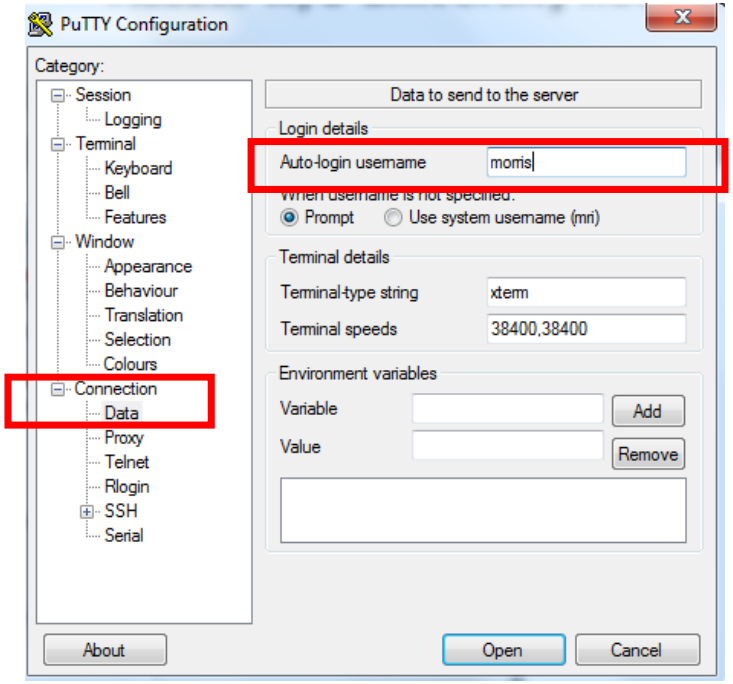
Using SSH to connect to HPC Systems



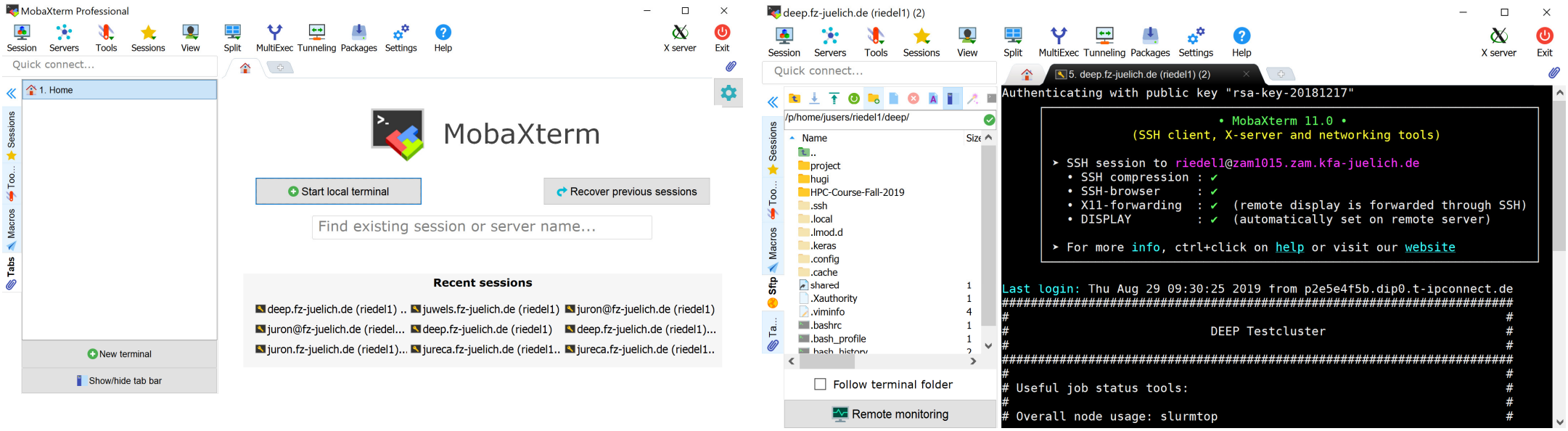
SSH Clients – Putty for Windows

- Example: Putty SSH Client for Windows
  - Not recommended, better install MobaXterm





MobaXterm SSH Client



[5] MobaXterm SSH Client

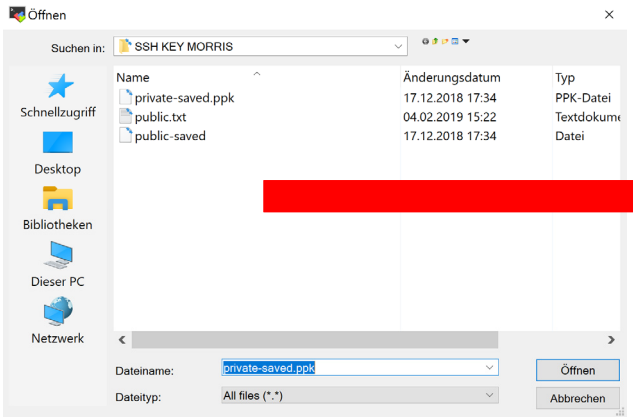
SSH Keys – Example Morris Public Key

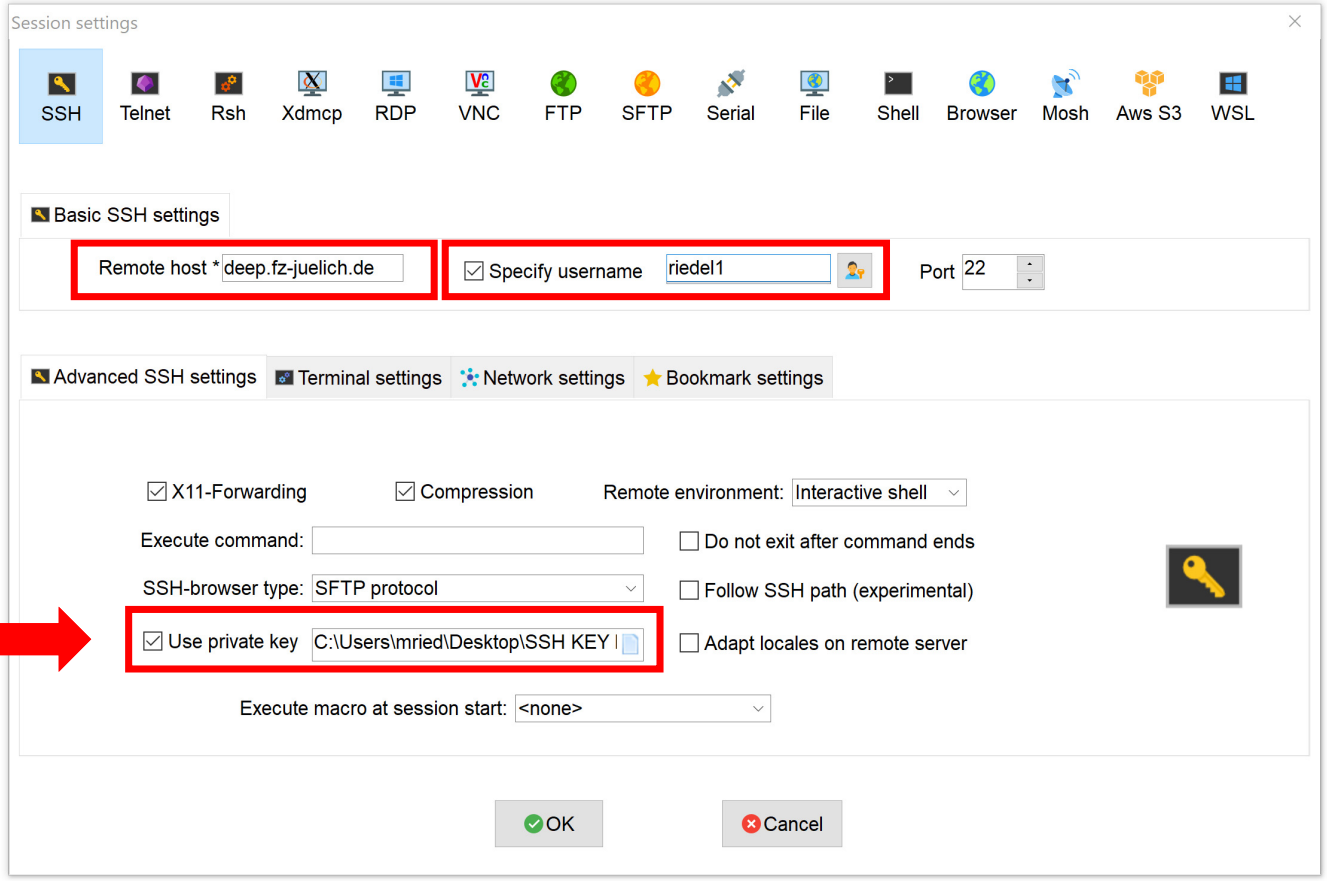
- Everybody is allowed to see the public key
  - Given to HPC administrators
  - Sometimes uploaded in Web forms
  - Only Morris has the corresponding private key that never leaves the laptop of Morris (!)

- SSH Key Example
  - ssh-rsa AAAAB3NzaC1yc2EAAAABJQAAAQEAruA2IJQmVEwVjsQ6N9PUJP0KukCGQV2yAMs3hop0stsvfb4Iac7s2PqkwOgoFPZGwRCSGcA2/rISJX3MxEmx7EQLD5sw63r8LqvETXy4hmefIlBwpcIxMBYSLujWdCH9K60Q6TApMz4hV+fsZRiGbTx7hs9Y2a3TiiSE032IvzxMYTvW8NYlhXOP9PzTR1jebVj3rgcOIYLPMGzl4YIbCZJVIeJlwfkZscOH9zT4Kl5SpQuk5Q+LyMl95X3xsk3xPMCuocqsYmIY6Gp+BCAYJsdCXFNDJ3SCcphziTqrE+F2EroI4AoegVlH/vhPaAZgQ222nV2rDsN+uDhaBf+76Q== rsa-key-20181217

SSH Keys – Use Private/Public Key Pair to Access DEEP HPC System

- Remember to use your Private SSH Key to connect to the DEEP system
  - Corresponding Public SSH key is already uploaded on the HPC System (remote host) per username(!)

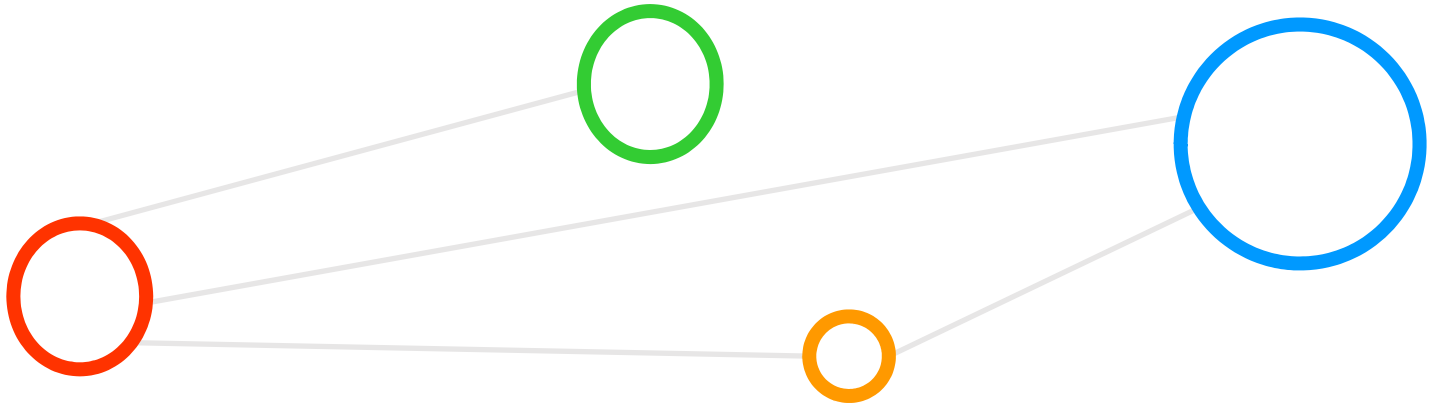




SSH Access to HPC Systems – DEEP HPC System Example

- HPC System Address
  - deep.fz-juelich.de
  - alias for zam1015.zam.kfa-juelich.de
- HPC System Username
  - Example: riedel1
  - Every student will get a different username
- HPC System Welcome Screen
  - If SSH login was succesful
  - Shows useful information about the system
  - E.g. status of the file system or known errors / bugs
  - E.g. help with important commands

Lecture Bibliography



Lecture Bibliography

- [1] Icelandic HPC Machines & Community, Online: http://ihpc.is
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