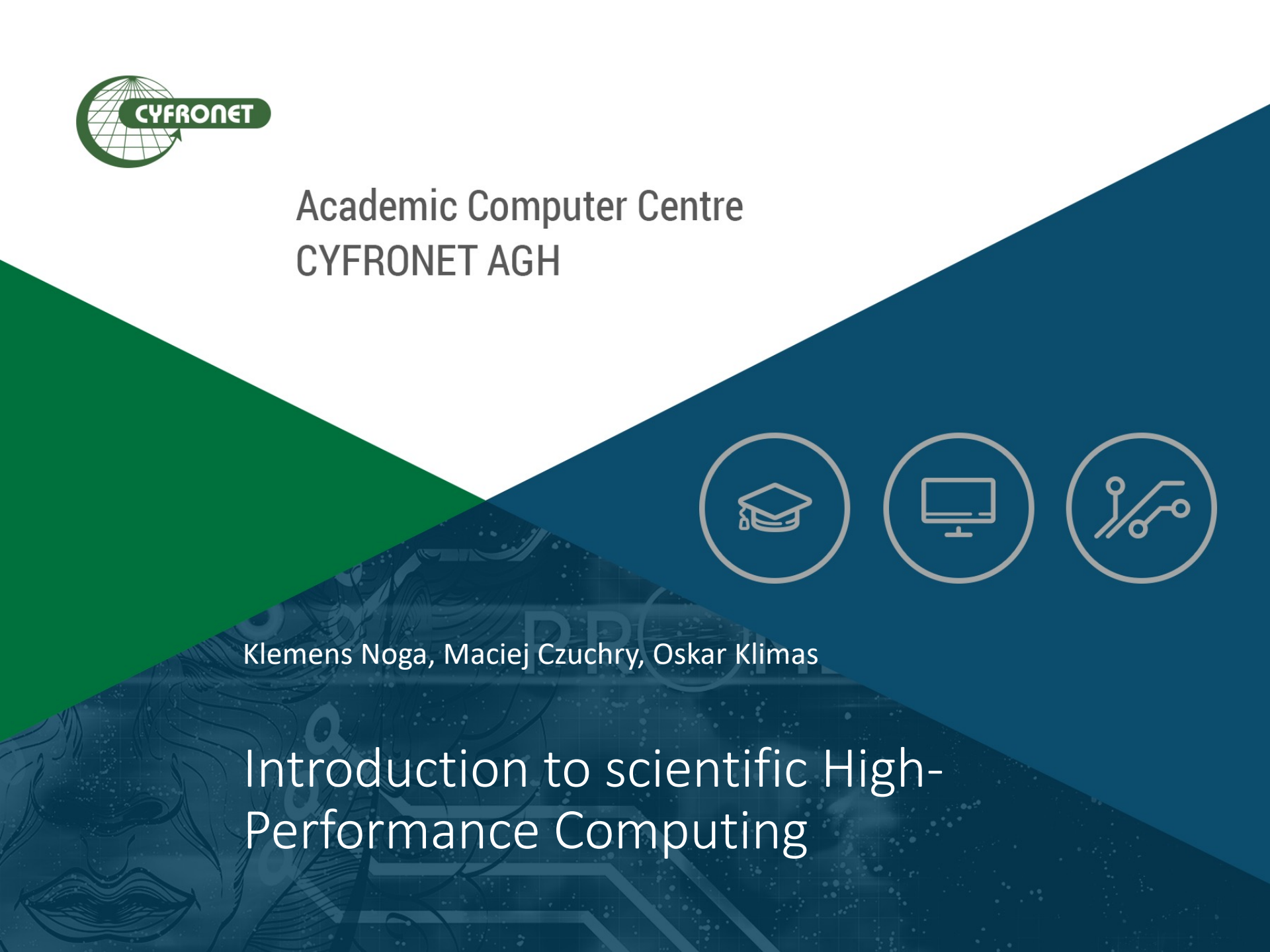


Academic Computer Centre
CYFRONET AGH

Klemens Noga, Maciej Czuchry, Oskar Klimas

Introduction to scientific High-Performance Computing

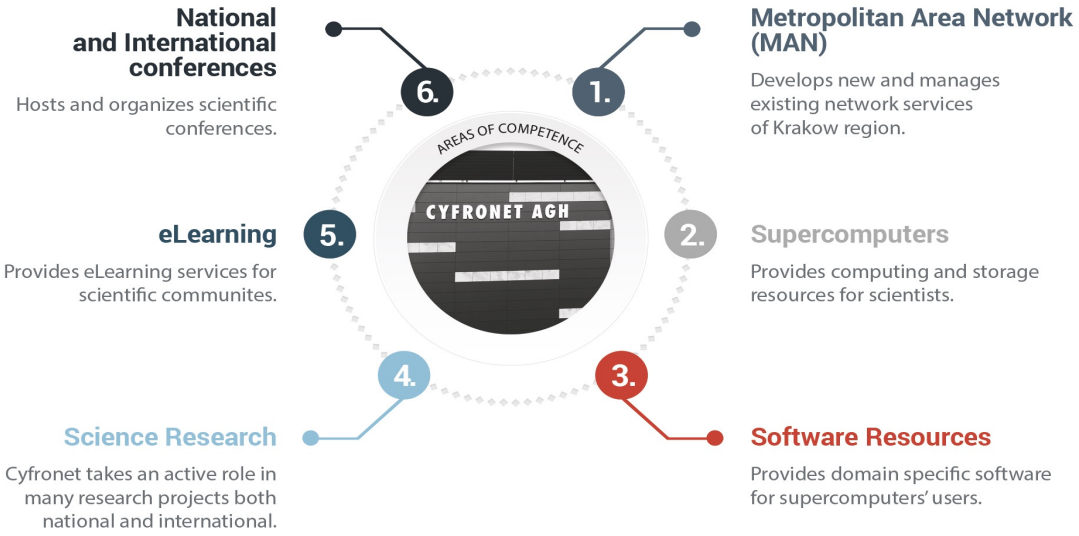
Agenda

- **Athena, Ares & Prometheus clusters at ACC Cyfronet AGH**
  - available resources
- **Accessing and working with HPC resources**
  - access to clusters/data transfer
  - command line interface
  - tasks automation
- **Documentation and users' support**
- **Questions and exercises**

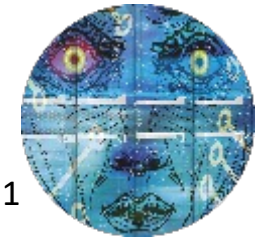
CYFRONET

Academic Computer Centre Cyfronet AGH

- The biggest Polish Academic **Computer Centre**
  - **50 years of experience** in IT provision
  - Centre of Excellence in **HPC, Grid and Cloud Computing**
  - Home for **Athena**, **Ares, Prometheus and Helios supercomputers**
  - **LUMI** consortium partner (EuroHPC pre-exascale supercomputer **#3 on TOP500**)
- Legal status: an **autonomous** within AGH University of Science and Technology
- Staff: 180+ , ca. 80 in R&D
- Leader of **PLGrid**: Polish Grid and Cloud Infrastructure for Science
- NGI Coordination in **EGI e-Infrastructure**



Prometheus



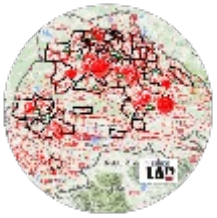
- 2.40 PFLOPS
- 53 568 cores
- From 2015 to 2021 1st HPC system in Poland (475th on Top 500, 38th in 2015)

Athena

- 7.71 PFLOPS
- 384 A100 GPGPUs
- 1st HPC system in Poland (since 2022, 105th on Top500)
- 9th on Green500

Ares

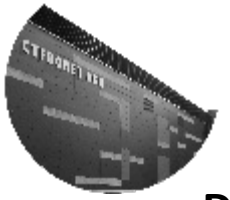
- 4.00 PFLOPS
- 38 112 cores
- 290th on Top 500



Computing portals and frameworks

- OneData
- PLG-Data
- Rimrock
- InSilicoLab

Storage



- 60+ PB
- hierarchical data management

Research & Development

- distributed computing environments
- computing acceleration
- machine learning
- software development & optimization

Data Centres

- 3 independent data centres
- dedicated backbone links

Computational Cloud

- based on OpenStack

- Supercomputers from Poland
  - 105 – Athena (ACC Cyfronet AGH) (PLGrid) (#9 on Green500)
  - 145 – Altair (PSNC) (PRACE-LAB)
  - 290 – Ares (ACC Cyfronet AGH) (PLGrid)
  - 462 – Tryton Plus (TASK) (PLGrid)
  - 475 – Prometheus (ACC Cyfronet AGH) (PLGrid)

TOP500 The List.

CYFRONET

- Supercomputers from Poland
  - 113 – Athena (ACC Cyfronet AGH) (PLGrid) (#17 on Green500)
  - 158 – Altair (PSNC) (PRACE-LAB)
  - 323 – Ares (ACC Cyfronet AGH) (PLGrid)

TOP500 The List.

CYFRONET

- Supercomputers from Poland
  - 123 – Athena (ACC Cyfronet AGH) (PLGrid) (#19 on Green500)
  - 186 – Altair (PSNC) (PRACE-LAB)
  - 362 – Ares (ACC Cyfronet AGH) (PLGrid)

TOP500 The List.

CYFRONET

- Supercomputers from Poland
  - 155 – Athena (ACC Cyfronet AGH) (PLGrid) (#22 on Green500)
  - 221 – Altair (PSNC) (PRACE-LAB)
  - 291 – Helios CPU partition (ACC Cyfronet AGH) (PLGrid)
  - 404 – Ares (ACC Cyfronet AGH) (PLGrid)

TOP500 The List.

CYFRONET

Cyfronet flagship HPC systems

- 2006 - Baribal, 384 GFLOPS
  - large SMP
- 2010 - Zeus, 374 TFLOPS
  - commodity cluster with multiple partitions
- 2015 - Prometheus, 2,4 PFLOPS
  - fastest system in Poland's history
- 2021 - Ares, 4,0 PFLOPS
  - innovative liquid cooling and heat re-use
- 2022 - Athena, 7,7 PFLOPS
  - fastest system in Poland for HPC and AI
- 2023 - Helios
  - ?

Phaeton – testbed HPC system

288 TFLOPS
HPC FP64

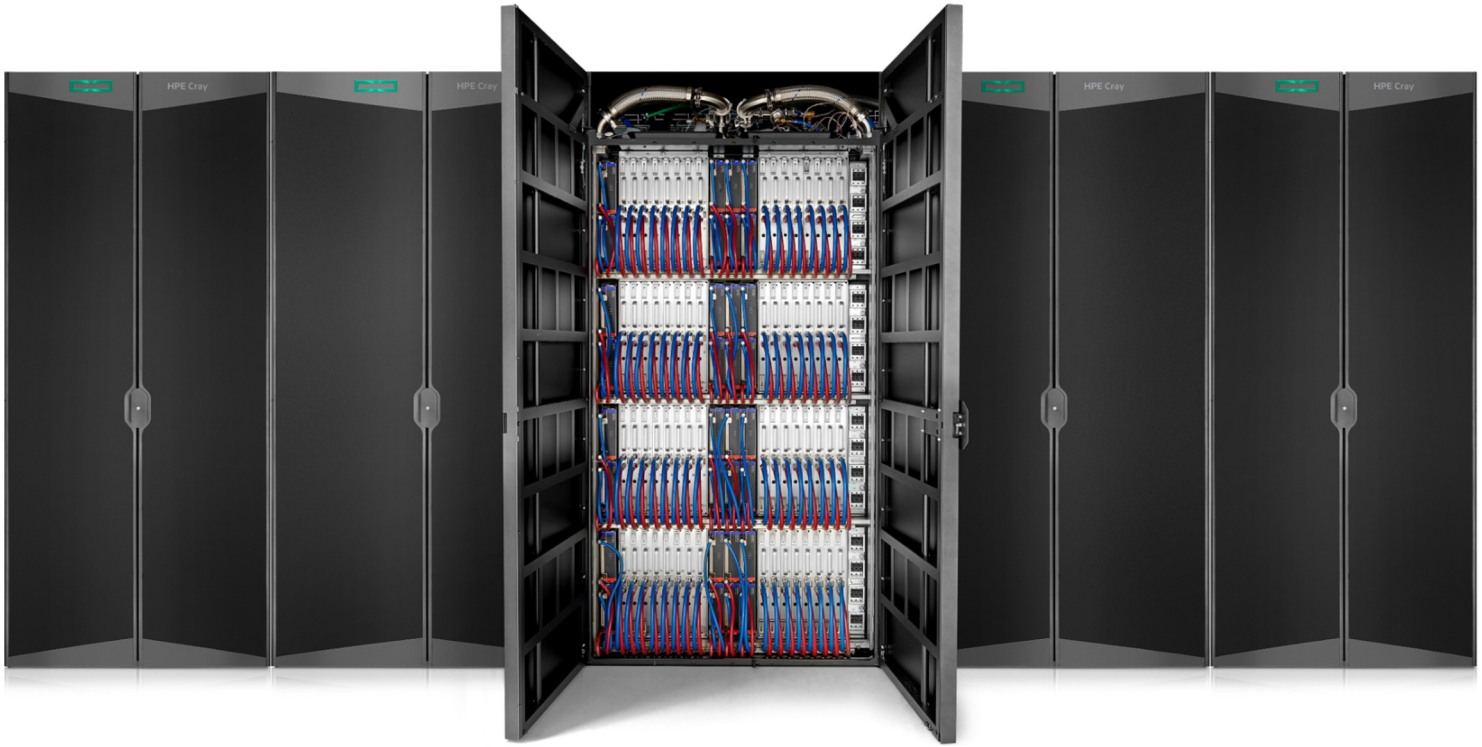
EuroHPC PL

CYFRONET

intel

- 60 Intel servers
  - 2x Intel Xeon 8352s, 1 TB RAM, 2x 100 GbE
- 4 large memory nodes
  - 2x Intel Xeon 8352s, 1 TB RAM + 8 TB Intel Optane, 2x 100 GbE
- 12 disk nodes
  - 2x Intel Xeon 8352s, 512 GB RAM + 1 TB Intel Optane, 100 TB NVMe
  - DAOS
- OS/Middleware:
  - Rocky Linux 9, Openstack, Openshift
- Main usage:
  - interactive work (pre- and postprocessing)
  - data analytics
  - front-end for HPC/AI services

CYFRONET

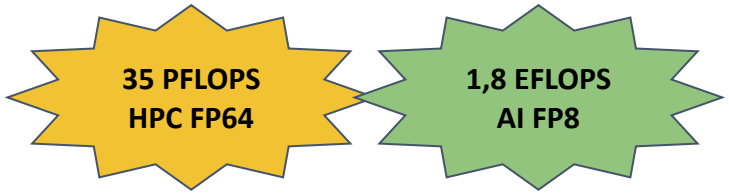

HPE Cray
HPE Cray
HPE Cray
HPE Cray

Announcing HPE Supercomputing Solution for Generative AI with NVIDIA Quad GH200

Hewlett Packard Enterprise | NVIDIA

CSCS Centro Svizzero di Calcolo Scientifico Swiss National Supercomputing Centre | CYFRONET | Los Alamos NATIONAL LABORATORY | NCSA | University of BRISTOL

Helios



EuroHPC PL

CYFRONET

- CPU partition (75264 cores, 196 TB RAM)
  - 272 standard nodes
    - 2x AMD 9654, 384 GB DDR5, 1x Slingshot 200 Gb/s
  - 120 nodes with double memory
    - 2x AMD 9654, 768 GB DDR5, 1x Slingshot 200 Gb/s
- GPU partition (440 accelerator modules)
  - 110 nodes
    - 4x NVIDIA Grace Hopper GH200 CPU+GPU, 4x Slingshot 200 Gb/s
- INT partition (24 accelerators)
  - 6 nodes
    - 2x AMD 9654, 1536 GB DDR5, 4x NVIDIA H100 HGX 94 GB, 30 TB NVMe, 2x Slingshot 200 Gb/s

AMD

NVIDIA

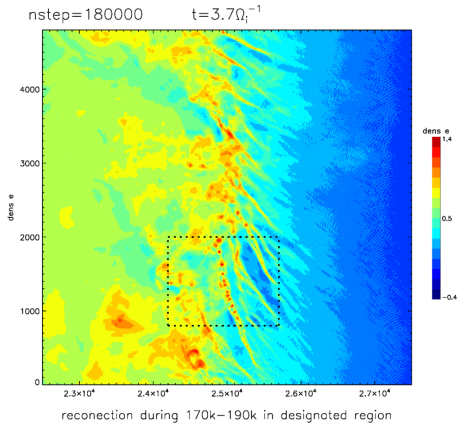
CYFRONET

Helios

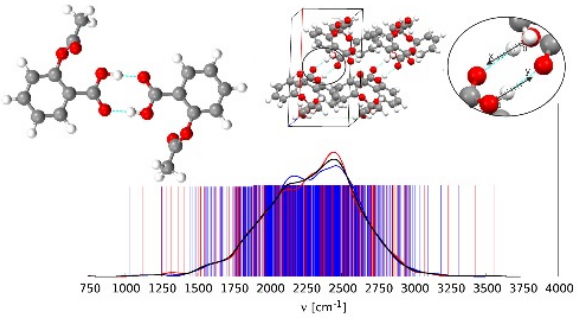
- HPE Cray EX4000
  - full direct liquid cooling
    - >99% energy to liquid
    - DLC for servers, switches, power supplies
    - up to 400 kW per rack
    - 3,5 tons per rack
  - Slingshot network
    - 200 Gb/s per port
    - low latency, RDMA, adaptive routing
    - compatible with Ethernet
  - platform used to build world's largest systems
    - Frontier, El Capitan, Aurora, LUMI, ALPS, Shaheen III, Setonix

Usage examples

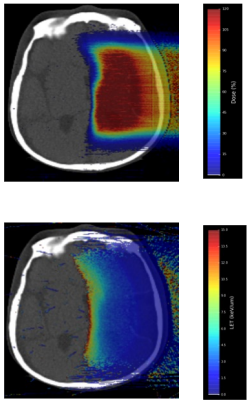
- Astrophysics: users' own code
  - Particle in Cell written in Fortran
  - Production runs - 9600 cores
    - One run up to 460 800 h CPU time – 53 years



- Chemistry: CPMD, CP2k, Jaguar, Gaussian
  - Importance of hydrogen bonds in biomolecules
  - Jobs: 24-240 cores
    - Hundreds of thousands of jobs with walltime < 1 h
    - Efficient usage resources through backfill

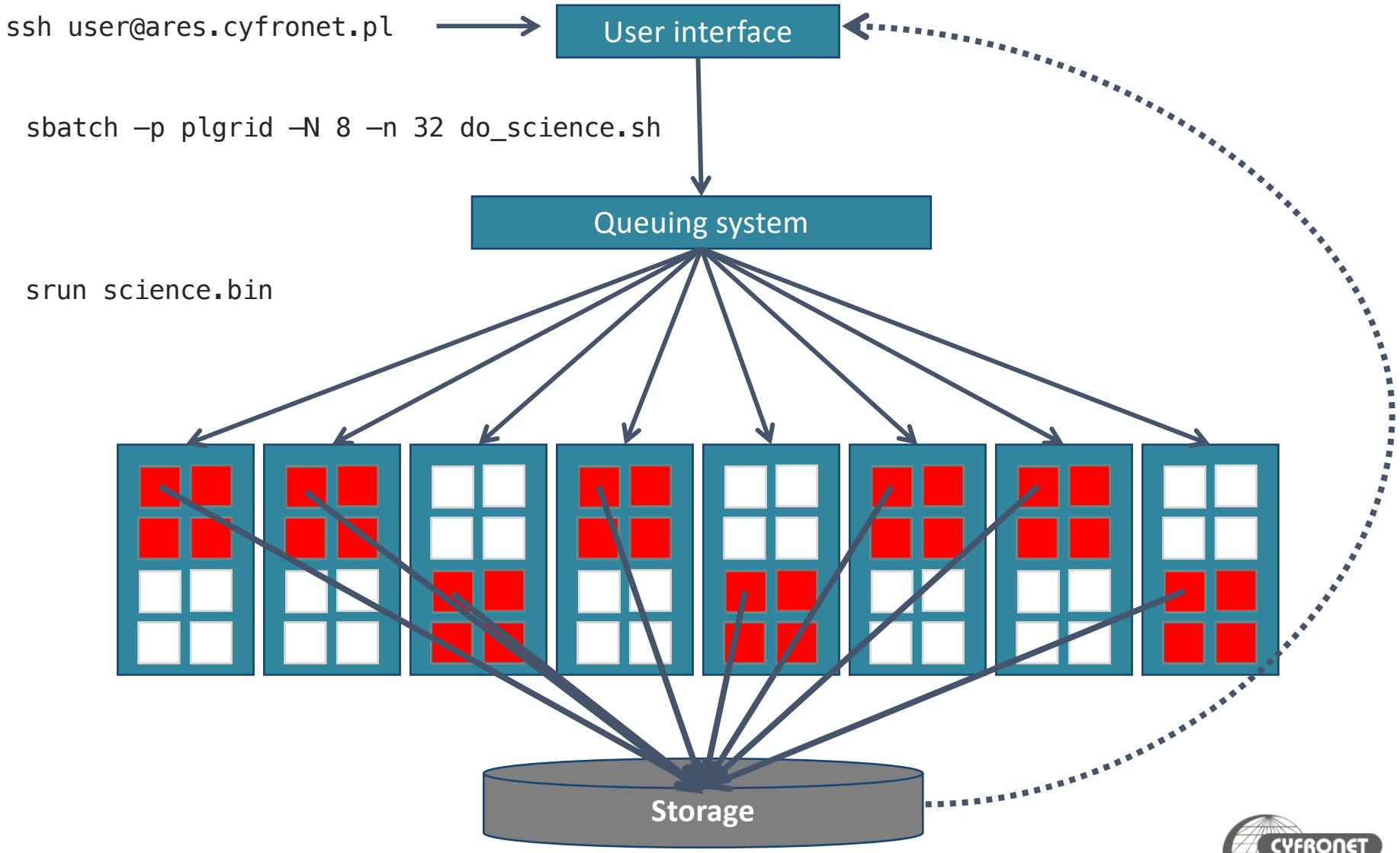


- Biophysics: Proton therapy
  - Monte Carlo simulations of a proton beam
  - Monte-Carlo based treatment planning
  - Jobs:
    - thousands of jobs with MC simulations (hours on hundreds of nodes)
    - Interactive large data processing with Jupyter noteboooks

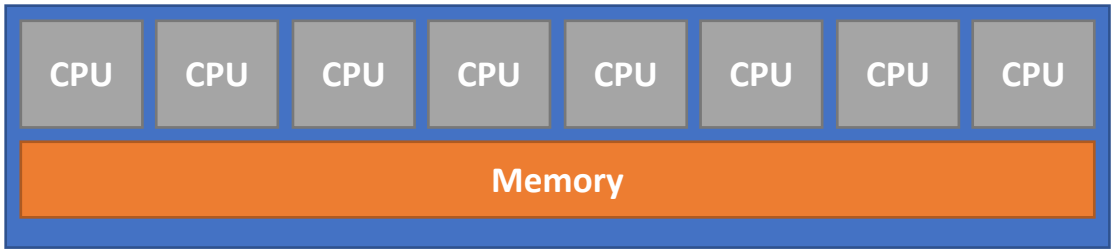


What is HPC?

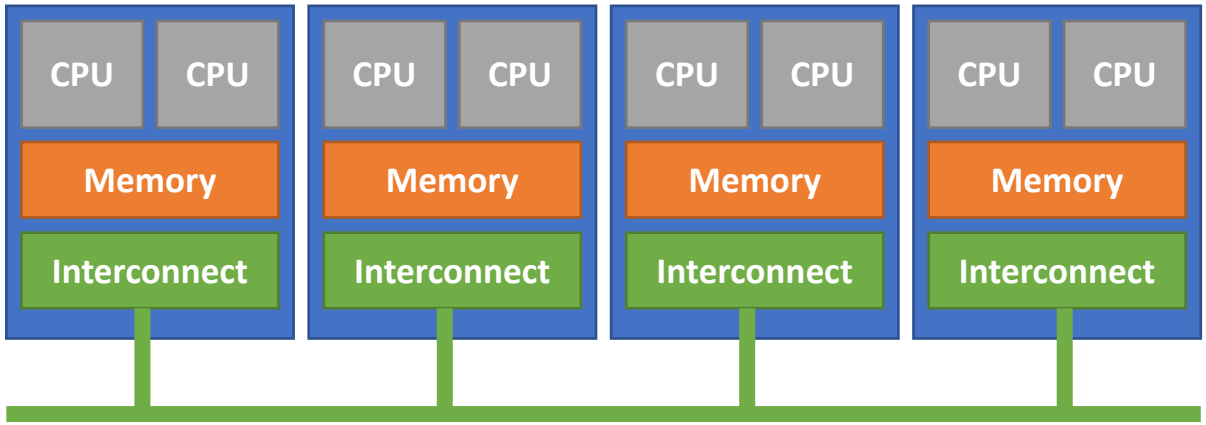
- High Performance Computing (HPC) – using supercomputers to solve problems that cannot be addressed by regular computes
  - use vast amount of processors/cores simultaneously
  - use huge memory allocations
  - use specialized computation accelerators (GPUs, FPGA, ASIC)
  - very fast access to data on dedicated high performance storage systems
- High Throughput Computing (HTC) – processing as much jobs (individual job could be quite simple) as possible using HPC infrastructure
- High Performance Data Analysis (HPDA) - using HPC infrastructure to analyse vast amount of data


ssh user@ares.cyfronet.pl
User interface
sbatch –p plgrid –N 8 –n 32 do_science.sh
Queuing system
srun science.bin
Storage

SMP


CPU
CPU
CPU
CPU
CPU
CPU
CPU
CPU
Memory

Cluster


CPU
CPU
Memory
Interconnect
CPU
CPU
Memory
Interconnect
CPU
CPU
Memory
Interconnect
CPU
CPU
Memory
Interconnect

Cyfronet/PLGrid - accessing resources

Steps necessary to grant access to Cyfronet/PLGrid resources

- Create account at PLGrid Users' Portal – https://portal.plgrid.pl
- Create (Scientific) Affiliation
- Create/Join Team
- Create Computational Grant for the team
- Apply for necessary services/entry points

Ares HPC cluster

- Ares consists user interface nodes (UI), service nodes and worker nodes
  - 788 CPU nodes (2x Intel Xeon Platinum 8268 processors, 48 x 2.9 GHz)
    - 532 nodes with 192 GB RAM (4GB/core)
    - 256 nodes with 384 GB RAM (8GB/core)
  - 9 ML/AI nodes (2 x Intel Xeon Gold 6242, 32 x 2.8 GHz, 384 GB, 8 x NVIDIA V100 SXM2 32GB HBM2)

Property	Ares	Ares GPU
CPU frequency	2.9 GHz	2.8 GHz
RAM	192/384 GB	384 GB
cores per node	48	32
InifiniBand interconnect	available, EDR 100 Gb/s	

Athena HPC cluster

- Ares consists user interface nodes (UI), service nodes and worker nodes
  - 48 GPGPU nodes (2 x AMD EPYC 7742, 64 x 3.3 GHz, 1 TB, 8 x NVIDIA A100 SXM2 40GB HBM2)

Property	Athena
CPU frequency	3.3 GHz
RAM	1024 GB
cores per node	128
InifiniBand interconnect	available, EDR 800 Gb/s

Access to computing clusters

- All PLGrid HPC clusters use Linux as OS
  - Rocky Linux on Ares and Athena
- HPC clusters contain
  - user interface (UI) node(s)
  - computing nodes (a.k.a worker nodes)
- User interface **must not be used** for computing
- Fair share between users' tasks and computations provided by queuing system
  - SLURM on Ares & Prometheus

Access to computing clusters

- User logs on user interface (UI) node using SSH protocol
  - UI names:
    - login@ares.cyfronet.pl
    - login@athena.cyfronet.pl
  - SSH clients
    - on Linux and MacOS included in OS
      - `ssh` command in terminal
    - on Windows
      - PuTTY - http://www.chiark.greenend.org.uk/~sgtatham/putty/
      - MobaXterm - http://mobaxterm.mobatek.net
      - Windows Terminal - https://aka.ms/terminal

Access to computing clusters

- User logs on user interface (UI) node using SSH protocol
  - copying files and directories
    - on Linux and MacOS included in OS
      - `scp` command in terminal
      - `rsync` command in terminal
    - on Windows
      - WinSCP - http://winscp.net/
      - Windows Terminal - https://aka.ms/terminal
        - `scp` command in terminal
        - `rsync` command in terminal
  - remote work
    - using CLI with `nano`, `vim`, `emacs`, `mc`
    - Visual Studio Code - https://code.visualstudio.com/
      - Remote – SSH extension
      - Remote – Tunnels
    - SSHFS via FUSE

Ares/Athena– file systems

- Storage of data – NFS (quite slow, should not be used for heavy I/O calculations)
  - `$HOME` – user's home directory
    - quota 10 GB
  - `$PLG_GROUPS_STORAGE` – additional storage gained through PLGrid grants system
- Temporary scratch file systems
  - `$SCRATCH` – distributed scratch Lustre file system
    - accessible from all nodes of cluster (including UI)
    - `$TMPDIR` and `$SCRATCHDIR` – unique subdirectories on `$SCRATCH` created for the job at it's start
- To check quota use `hpc-fs`

Software

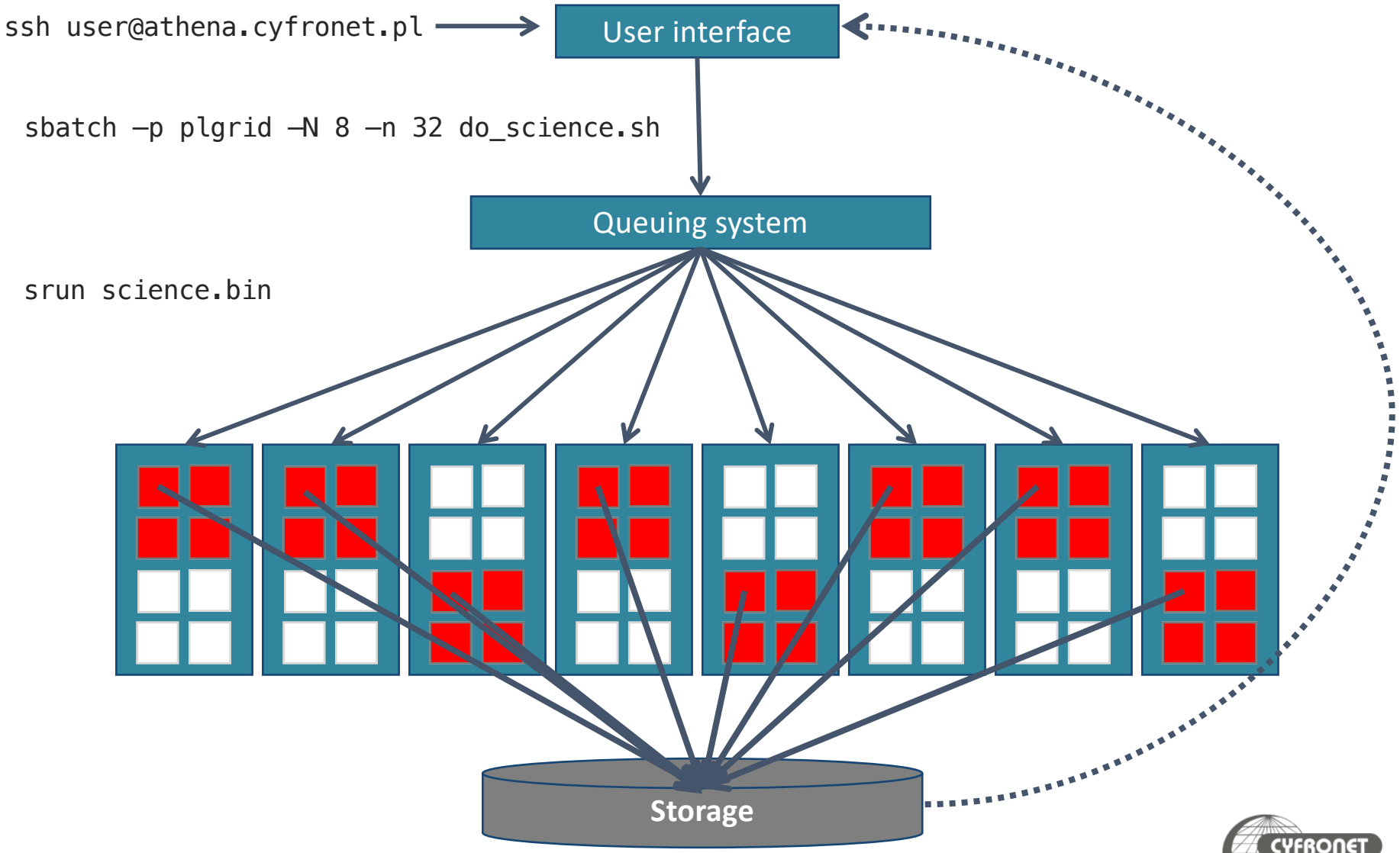
- Scientific software usually needs specific runtime environment (i.e. additional libraries) and sometimes technical knowledge is needed to install them efficiently
- Modules and Lmod packages are solutions for loading runtime environments on every cluster in PLGrid infrastructure
- Advantages
  - simplicity of preparing software to run efficiently
  - computation scripts could be transferable between HPC clusters
  - possibility of concurrent runs of different versions of software
  - on hybrid HPC systems transparent switching to most efficient version of software
- Drawbacks
  - additional command to remember .-)

Software – modules

- Load environment for scientific package
  - `module add <module-name>` (i.e. `module add plgrid/apps/r`)
  - `module load <module-name>` (i.e. `module load plgrid/apps/matlab`)
- Remove module
  - `module rm <module-name>` (i.e. `module rm plgrid/apps/r`)
  - `module unload <module-name>` (i.e. `module unload plgrid/apps/matlab`)
- Listing of all available modules
  - `module avail`
  - `module avail plgrid/tools` (only from `tools` branch)
  - `module avail plgrid/apps/r` (all available R versions in `plgrid/apps`)
  - `module spider python` (all available Python versions)
  - `module spider "/r/"` (all available R versions, regexp search)
- Listing of loaded modules
  - `module list`

Software – modules

- Clearing all loaded modules
  - `module purge`
- Saving collection of modules for later use, restoring it and listing saved collections
  - `module save [collection]`
  - `module restore [collection]`
  - `module savelist`
  - `module describe [collection]`
- `ml` is shorthand for `module` command
  - `ml = module list`
  - `ml <module-name> = module load <module-name>`
  - `ml -<module-name> = module unload <module-name>`
  - `ml av <string> = module avail <string>`
- Getting help
  - `module help`
  - `ml -h`


ssh user@athena.cyfronet.pl
User interface
sbatch –p plgrid –N 8 –n 32 do_science.sh
Queuing system
srun science.bin
Storage

SLURM queuing system – commands

- User interact with SLURM queuing system using commands
  - `sbatch` – to submit new job to queue
  - `squeue` – gives information about jobs running in queuing system
  - `scancel` – deletes jobs from queue
  - `sinfo/scontrol` – gives detailed information about queue, job or node
  - `smap` – gives graphical information about state of HPC cluster
  - `srun` – runs interactive job or step in batch job

- Each job has got **unique job identifier** (jobID)

Queuing system

- Queuing system
  - manages all computational task on cluster
  - monitors available resources
  - acts as matchmaker between needs of jobs and resources
  - empowers fair share between different users

- All computational tasks are run as **jobs** queued in **queues** and run according to their priority and available resources.
- Priority of job depends on
  - amount of resources obtained by user in computational grant
  - amount of resources requested by job
    - **maximum wall time of computation** is most essential resource
  - amount of other resources concurrently used by job's owner

Queuing systems in PLGrid

- HPC clusters available in PLGrid use several kinds of queuing systems
  - SLURM (http://slurm.schedmd.com)
  - PBS Pro (http://pbspro.org)

HPC Centre	Cluster	Queuing system
ACC Cyfronet AGH	Prometheus	SLURM
	Ares	SLURM
	Athena	SLURM
PSNC	Eagle/Altair	SLURM
TASK	Tryton	SLURM
WCSS	Bem	PBS Pro
	Bem2	SLURM

SLURM queuing system – job submission

- Command `sbatch` submits new job in queue
- All parameters describing job's requirements could be included in batch script and given to queuing system using command
  - `sbatch [options] script.slurm`
- Example script

```
#!/bin/env bash

# Commands that will be run after start of the job
echo "Computation started on work node: ";
hostname

module add matlab

matlab –nodisplay <matlab.in >matlab.out
```

SLURM queuing system – job monitoring

- Commands `squeue` and `hpc-jobs` give view of jobs scheduled in queuing system
- Jobs States
  - `PD` – queued
  - `R` – running
  - `CF` – configuring (resources for job are being prepared)
- Additional helpful flags
  - `squeue --user $USER` – information about `$USER`'s jobs
  - `hpc-jobs -j <jobID>` – information about specified jobs
  - `hpc-jobs -N` – additional information about information about exec nodes
  - `hpc-jobs -q/-r` – information about queued (pending)/running jobs only
  - `hpc-jobs -h` – help screen
- In addition `scontrol`, `sinfo` and `smap` give information about status of cluster
  - `scontrol show job <jobID>` – information about `<jobID>` job
  - `scontrol show node <nodes_list>` – information about nodes

Available partitions

Partitions	max time	Information
plgrid-testing	1:00:00	for test runs (small number of jobs)
plgrid	3-00:00:00	
plgrid-now	12:00:00	interactive runs, max one job on one node
plgrid-long	7-00:00:00	*
plgrid-gpu	3-00:00:00	nodes with GPGPU*
plgrid-gpu-v100	1-00:00:00	nodes with V100 GPGPU*
plgrid-gpu-a100		nodes with A100 GPGPU*
plgrid-bigmem	3-00:00:00	big mem nodes*
plgrid-services	14-0:00:00	running “long-living” services*

- In SLURM queues are called partitions
- `scontrol show partitions <patition_name>` – detailed information about partition
- `sinfo` – lists all available nodes in all partitions
  - `sinfo –p <partition_name>` – lists information only about partition
- default time in all `plgrid*` partitions is set to 15 minutes

* - partitions available after request through PLGrid grants

SLURM – example Python job


```
#!/bin/env bash

# Commands that will be run after start of the job
echo "Computation started on work node: "; hostname

module add python

./python-script.py > python.log
```

- SLURM options provide information about job requirements to queuing system. They could be
  - given in command line `sbatch [SLURM options]`
  - included in first lines of batch script with `#SBATCH` at start of line

SLURM – `sbatch` command options

- `sbatch` command uses various options to provide queuing system with additional info about the job
  - `-p <partition>, --partition=<partition>` defines partition
  - `-J <jobname>, --job-name=<jobname>` give name to job
  - `-a, --array=<indexes>` submit a job array
  - `--mail-user=<user's e-mail>` setting email for notifications
  - `--mail-type=<type>` information when notifications should be send: at beginning (`BEGIN`), end (`END`) or execution error (`FAIL`)
  - `-A <grantID>, --account=<grantID>` information about computational grant (if omitted job use default)

- When option `-p` is omitted job is queued into default partition (on Prometheus `plgrid`)

SLURM – job requirements specification

- There are several recourses available for job
  - `-t, --time=<time>` total maximal execution wall time of job
  - `-N, --nodes=<nodes>` number of nodes allocated to job
  - `-n, --ntasks=<ntasks>` number of tasks invoked in whole job
  - `--ntasks-per-node=<ntasks>` number of tasks invoked on each node
  - `--cpus-per-task=<cores>` number of cores per each task (i.e., when using threads in OpenMP)
  - `--mem=<MB>` amount of memory per node requested by job
  - `--mem-per-cpu=<MB>` amount of memory per core requested by job

- Parameter formats
  - time format: `"min", "min:sec", "hours:min:sec", "days-hours", "days-hours:min" and "days-hours:min:sec"`
  - memory: `MB (=1024kB), GB (=1,024MB)`

SLURM – example serial job


```
#SBATCH --job-name=serial.job
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --time=10:00
#SBATCH --mem=24000
#SBATCH --partition=plgrid
#SBATCH --account=tutorial

module add intel

icc -xHost hello.c -o hello.x

./hello.x
```

- In SLURM job is sent to partition not to queue
  - flag `-p <partition_name>` or `--partition <partition_name>`
  - partition for PLGrid users: `plgrid*`

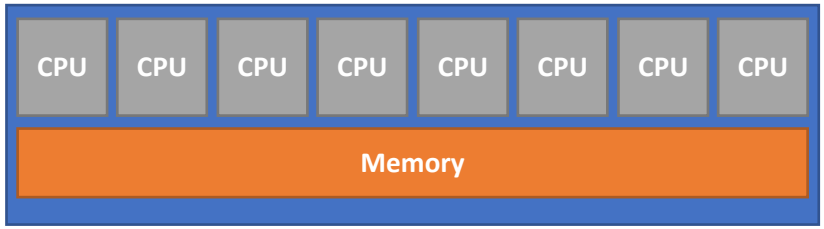
SLURM – example parallel job


```
#SBATCH --job-name=parallel-srun
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=2
#SBATCH --time=10:00
#SBATCH --mem-per-cpu=1GB
#SBATCH --partition=plgrid
#SBATCH --account=tutorial

module add intel

icc -xHost hello.c -o hello.x

srun ./hello.x
```

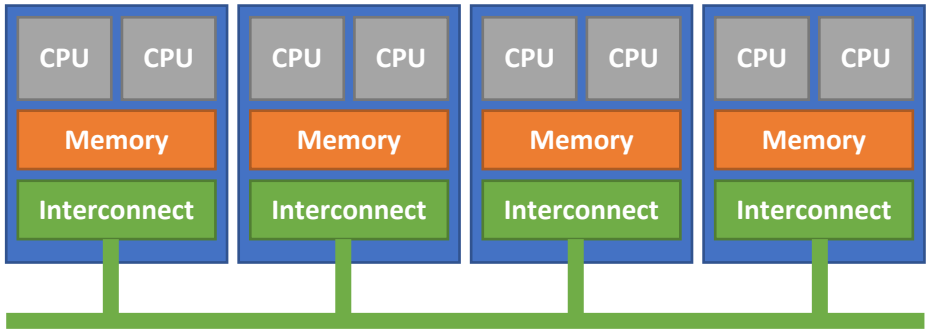
- `srun` inside batch job executes command `./hello.x` on allocated resources according to `requested --ntask` or `--nodes*--ntasks-per-node` flags
  - variable SLURM_NTASKS holds information about number of tasks to be run
- each `srun` could request more than one core
  - `srun –nodes=x --ntasks=y --cpus-per-task=z …`

- OpenMP
  - API for writing shared-memory software
  - Shared memory in threads
  - Requires support in compiler (-qopenmp, -fopenmp)
- MPI
  - Message Passing Interface (send, receive, broadcast)
  - Every process has its own isolated memory space
  - Can use more than one machine via interconnect (eth, infiniband)

SMP



Cluster



SLURM – example parallel OpenMP job


```
#SBATCH --job-name=parallel-openmp
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=12
#SBATCH --time=10:00
#SBATCH --mem-per-cpu=2GB
#SBATCH --partition=plgrid
#SBATCH --account=tutorial

module add intel

icc -xHost -qopenmp hello.c -o hello.x

export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

./hello.x
```

- When use OpenMP
  - use `--cpus-per-task=<cores_per_job>` and `--nodes=1` for request of resources
  - variable `SLURM_CPUS_PER_TASK` holds information about number CPUs allocated to each task

SLURM – example parallel MPI job


```
#SBATCH --job-name=distributed-mpi
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=12
#SBATCH --time=10:00
#SBATCH --mem-per-cpu=1GB
#SBATCH --partition=plgrid
#SBATCH --account=tutorial

module add iimpi

mpiicc -xHost hello.c -o hello.x

mpiexec -np $SLURM_NTASKS ./hello.x
```

- When software is parallelized using MPI
  - use `--ntasks-per-node=<cores_per_node` and `--nodes=<no_of_nodes>` for request of resources
  - variable `SLURM_NTASKS` holds information about number of tasks to be run

SLURM – example parallel hybrid MPI/OpenMP job


```
#SBATCH --job-name=mpi-openmp
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=4
#SBATCH --cpus-per-task=6
#SBATCH --time=10:00
#SBATCH --mem-per-cpu=2GB
#SBATCH --partition=plgrid
#SBATCH --account=tutorial

module add iimpi

mpiicc -xHost -qopenmp hello.c -o hello.x

export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

mpiexec -np $SLURM_NTASKS ./hello.x
```

- When hybrid MPI/OpenMP
  - use `--cpus-per-task=<cores_per_job>` and `$SLURM_CPUS_PER_TASK` for distribution of threads
  - use `--ntasks-per-node=<cores_per_node>` for request of MPI processes
  -

SLURM – environmental variables

- SLURM adds environmental variables which could ease performing computation

Variable	**Description**
SLURM_JOB_ID	job identifier (jobID)
SLURM_SUBMIT_DIR	dir, from which batch script was submitted to queuing system
SLURM_NTASKS	total number of tasks (i.e. MPI processes) in the current job
SLURM_NTASKS_PER_NODE	number of tasks to be run on one node
SLURM_NODELIST	list of nodes allocated to the job
SLURM_CPUS_PER_TASK	number of cores requested per task
SCRATCH	$USER's root scratch directory on distributed Lustre file system
SCRATCHDIR	unique directory for the job on $SCRATCH

- Environment variables can be used to control distribution of job
  - MPI jobs: SLURM_NTASKS to run MPI processes (using `srun`) variable
  - OpenMP jobs: SLURM_CPUS_PER_TASK to run proper number of threads
  - hybrid MPI/OpenMP jobs: combine SLURM_NTASKS to run MPI processes and SLURM_CPUS_PER_TASK to expand threads

SLURM – interactive jobs

- Interactive work on cluster should be done using interactive jobs trough `srun` command
  - `srun -p plgrid -A <grant_id> -n 1 --pty /bin/bash`
- User interface **must not be used** for computing
- High priority queue `plgrid-now` for interactive work
  - one job on one node up to 12:00:00
- To attach terminal to running batch job
- `srun -N1 -n1 --jobid=<jobID> --pty /bin/bash`
- `srun -N1 -n1 --jobid=<jobID> -w <nodeID> --pty /bin/bash`
- `sattach <jobid.stepid>`
- Helper script `ssh_slurm`
  - `ssh_slurm <jobid> <dest_host> [command]`

SLURM `scancel` – deleting jobs

- `scancel` command is used to delete unwanted jobs from queuing system
  - `scancel <JobID>`

- Information about jobs which cannot be deleted using `scancel` should be sent to system administrators through
  - Helpdesk PLGrid PL
    - https://helpdesk.plgrid.pl
    - helpdesk@plgrid.pl
  - directly to system administrators prometheus@cyfronet.pl

Job monitoring with `hpc-jobs*`

- `hpc-jobs` and `hpc-jobs-history` could be used to monitor efficiency of jobs
  - memory usage
  - CPU usage

- `hpc-jobs` – running and queued jobs
- `hpc-jobs-history` – historical data of completed jobs

- `hpc-jobs*` usage
  - `hpc-jobs -N` – additional information about nodes of job(s)
  - `hpc-jobs -v` – more detailed information about job(s)
  - `hpc-jobs -j (<jobID>)` – information only about job(s)
  - `hpc-jobs -h` – help screen
  - `hpc-jobs-history -d <period>` jobs completed in last <period> days

Computational grants

- Obtained through PLGrid Portal - https://grants.plgrid.pl/
  - distinct allocations for CPU, GPGPU and storage with suffixes (`–cpu`, `–gpu` etc.)
- Information about grants from CLI
  - `hpc-grants`
- Cost of job
  - CPU only – in CPU-hours

```
cost_cpu    = job_cpus_used * job_duration
cost_memory = ceil(job_memory_used/memory_per_cpu) * job_duration
final_cost  = max(cost_cpu, cost_memory)
```

  - GPU – in GPU-hours

```
cost_gpu    = job_gpus_used * job_duration
cost_cpu    = ceil(job_cpus_used/cpus_per_gpu) * job_duration
cost_memory = ceil(job_memory_used/memory_per_gpu) * job_duration
final_cost  = max(cost_gpu, cost_cpu, cost_memory)
```

Best practices

- SLURM job batch script is always started in directory from which it was submitted to queuing system. Access to that directory is also possible with `SLURM_SUBMIT_DIR`

- All batch jobs have got file in which data from standard outputs (both standard output stream `stdout` and standard error stream `stderr`) is stored named `slurm-<JobID>.out`
  - those file should not be big (less than several MBs) and are stored in `SLURM_SUBMIT_DIR`
  - `-o, --output=<file>` and `-e, --error=<file>` - options to redirect `stdout` and `stderr`

- When commands in SLURM script print big amount of data into output streams user should redirect that data to file(s)
  - for standard output stream (*stdout*): `command > file.out`
  - for standard error stream (*stderr*): `command 2> file.err`
  - for both streams to one file: `command &> file.log`

- `$HOME` and `$PLG_GROUPS_STORAGE` **must not be used** for heavy I/O computations

Best practices

- During batch job submission user should always
  - specify maximal time of job execution (parameter `t/time`)
  - specify maximal RAM amount needed by job through `mem` (or `mem-per-cpu`)
  - enable checkpoints
  - for parallel computations use all cores on nodes when possible
  - when big amount of data is used in computation always use `$SCRATCH` for files
  - when big amount of data is going to be passed to standard output streams redirect it to files and use `$SCRATCH`
  - load runtime environment of software via `module` command in batch script
  - do not load software modules in scripts loaded at user's login (i.e. `.bashrc`)

Best practices – scalability tests

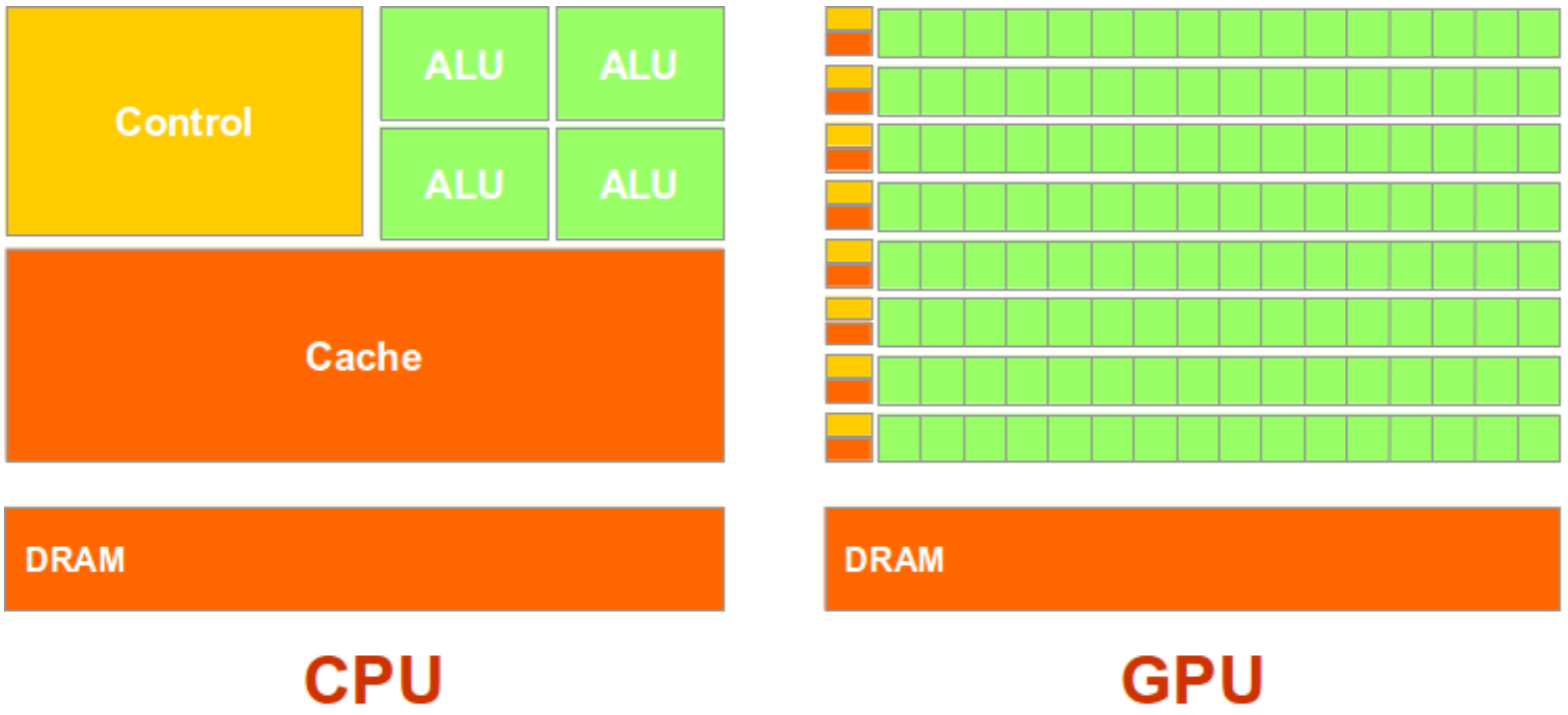
- Before start of big computations do scalability tests
  - Start from one quarter of node or one NUMA-node and scale up
  - Check computations efficiency with hpc-jobs/hpc-jobs-history and performance tools available internally in your software
- From SLURM scheduler point of view
  - If the job can scale with reasonable efficiency up to a certain point where the job takes 1 day to execute, this is the best option.
  - As a general guideline, keeping job runtime from 1 hour to 3 days maximum is best. Too short jobs might result in significant scheduling overhead.

Additional „filesystems”

- MEMFS
  - `-C memfs`
  - `$MEMFS`
  - use memory as filesystem (120GB max)
    - Accessible only within node
  - available during JOB and lost after it finishes

- LOCALFS
  - `-C localfs`
  - `$SCRATCH_LOCAL`
  - use file as filesystem (512GB per node)
  - Each node has its own file! (not a shared filesystem)
    - Accessible only within node
  - Available during JOB and lost after it is finished

GPU vs CPU



David B. Kirk and Wen-mei W. Hwu, Programming Massively Parallel Processors

GPU vs CPU

- CPU
  - Universal
  - Complex logic, big managing part
  - Few concurrent threads
  - Big/multi-level cache memory hides latency of access to main memory
- GPU
  - Efficient in case of highly parallel workloads
  - Minimal managing part, main part of silicone – ALU and registers
  - vast amounts of concurrent threads
  - Multithreading hides latency of access to main memory

SLURM – jobs with GPGPUs

- GPGPUs are shown in SLURM queuing system as generic resources (GRES) with `gpu` identifier.
- To check where GPGPUs are available
  - `sinfo -o '%P || %N || %G'`
- To request GPGPUs for a job `--gres=gpu[:count]` or `--gpus=` has or to be added to sbatch/srun command
  - `srun -p plgrid-gpu -N 2 --ntasks-per-node=24 -n 48 -A <grant_id> --gres=gpu[:count] --pty /bin/bash -l`
  - `#SBATCH --gres=gpu[:count]`
- GPGPUs are available only in `plgrid-gpu-v100` and `plgrid-gpu-a100` partitions
- GPGPU available for job are listed in `$CUDA_VISIBLE_DEVICES` variable
- Usage of GPGPU could be check using `nvidia-smi`

SLURM – example gpu job


```
#SBATCH --job-name=serial.job
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --gpus=1
#SBATCH --time=10:00
#SBATCH --mem=24000
#SBATCH --partition=plgrid-gpu-v100
#SBATCH --account=tutorial

module add cuda

nvcc hello.cu -o hello.x

./hello.x
```

- Pro-viz is a new service for users of Prometheus that allows running GUI mode of software using: TurboVNC https://www.turbovnc.org or web browser
- To run TurboVNC, you have to install Java JRE x86.
- In first step user need to run pro-viz on the cluster. To use it you need to load software module of pro-viz:

```
module load pro-viz
```

Pro-Viz command syntax


```
      pro-viz ...
        start [-n CORES | -N NODES | -p PARTITION | -t TIME | -A
ACCOUNT | -r RESERVATION | -g GPUS | -C constraints | -m EMAIL-ADDRESS
] - start a new batch session
        interactive [ -p PARTITION | -t TIME | -A ACCOUNT | -r
RESERVATION | -g GPUS | -C constraints  ] - start a new interactive
session
        list - list all sessions
        attach JOBID - attach session to a working job with JOBID
        password JOBID - generate access token for session JOBID
        stop JOBID - terminate session JOBID
        killall - terminate all sessions
        help - duh
```

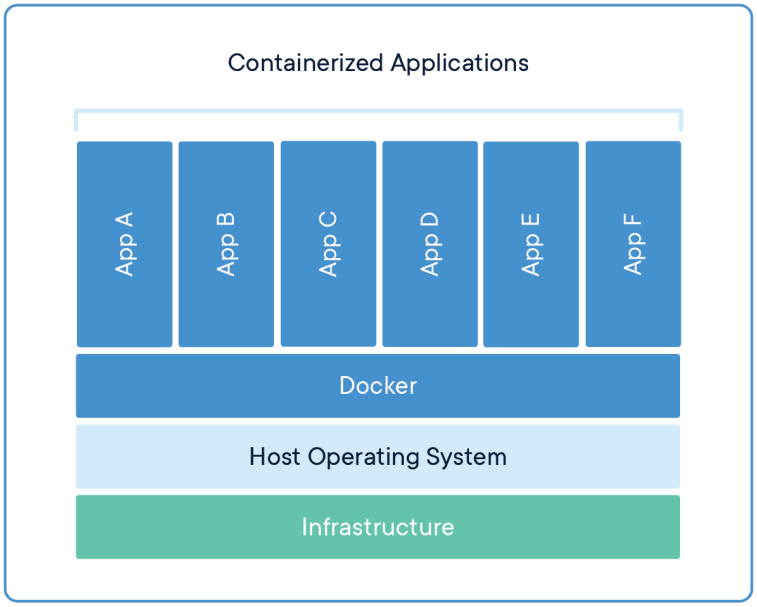
Pro-Viz command syntax

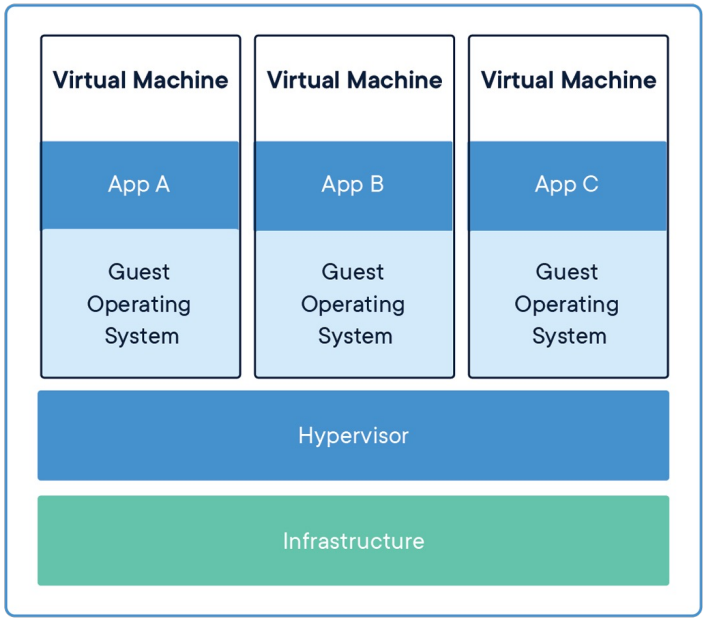
To start GUI session on cluster Ares with
12 cores on one node working node use commands:

- `module load pro-viz`
- `pro-viz start -N 1 -n 24 -p plgrid -A tutorial -t 03:00:00`
- `pro-viz password JOBID`

What is a container?

- A container is similar in purpose to a virtual machine (VM), providing encapsulation for a software application and it's runtime environment.
- Implementation differs. Containers use the host linux kernel instead of virtualizing hardware, so they are lightweight compared to VMs.
- Linux Containers rely on kernel features, and are inherently Linux based





Why use containers on HPC?

- Containers give Portability, Reproducibility, Scalability
  - Build once, use by many on many systems
    - Could move software stack to other HPC system
  - Isolate from changes in the HPC software environment
  - Save simulation/analysis software runtime for reproducible science

Singularity/Apptainer

- Usage
  - `singularity exec <container-name.sif> command`
  - `apptainer exec <container-name.sif> command`
  - `apptainer shell <container-name.sif>`
  - `apptainer run <container-name.sif>`
- Remarks
  - Possibility pull Docker/Singularity container

    ```
    apptainer pull docker:<repository>/<name-of-container>
    ```

  - Usage of GPU though –nv flag
  - Attach HPC system folders using –B flag, i.e:

    ```
    apptainer exec –B /net biopython_latest.sif python3

    apptainer exec –B $SCRATCH:/tmp/scratch biopython_latest.sif
    ```

- Usage restrictions
  - Creation of container requires root permissions, therefore cannot be done on HPC resources – use PLGrid cloud/your own resources instead

Singularity/Apptainer

- Additional Remarks
  - Use environmental variables to speed up converting containers
    - `APPTAINER_TMPDIR=$SCRATCHDIR or $MEMFS`
    - `APPTAINER_CACHEDIR=$SCRATCHDIR or $MEMFS`
  - Use $MEMFS filesystem to speed up I/O operations
  - Set working dir using `--pwd` option
  - Store data or datasets on $PLG_GROUPS_STORAGE/<your-team> or $SCRATCH
  - To use MPI you have to have compatible MPI flavours in the container and on the HPC system
    - Usually best solution is to have the PMI library in SLURM and start the container using `srun`

      srun --mpi=pmi2 `singularity exec …`

Python – package manager (pip)

- In Python you can easily manage your python modules via `pip` (`pip3`)
  - `pip list`
  - `pip search numpy`
  - `pip install numpy`
  - `pip install –U numpy`
  - `pip install –u numpy==1.10.1`
- The problem is when you need more than one environment
- Solution is virtualenv
  - `virtualenv --system-site-packages my_new_env`
  - `source my_new_env/bin/activate`
  - `pip install –U` whatever you want
  - `deactivate`
- One directory for each environment – clean project management

`python`

- Versions available at Ares cluster
  - GNU:
    - `2.7.x, 3.7.x, 3.8.x, 3.9.x, 3.10.x`
    - `python`
    - `python-bare` (minimal installation)
  - Additional libraries in in modules `scipy-bundle, ipython,` ect.

- Usage
  - `module add python/<version>`

- Remarks
  - Build with MKL numerical libraries, support for GPGPU computing

- Usage restrictions
  - only SMP mode (up to 48 computing cores@Ares)
    - multi-node MPI only with libs such as py4mpi , dask i.e.

Jupyter notebooks

- On HPC clusters, computations are executed on worker nodes
  - usually no GUI
  - usually behind firewall
- Jupyter notebook/Jupyterlab needs GUI in a web browser

- Therefore, there is a need to port tunnelling
  - First, submit job which creates Jupyter notebook and tunnel from worker node to login node
  - Establish tunnel from your computer to login node of cluster
  - Open notebook in your favourite browser on your computer

Jupyter notebooks

- SLURM job create
  - Jupyter notebook
  - tunnel from worker node to login node

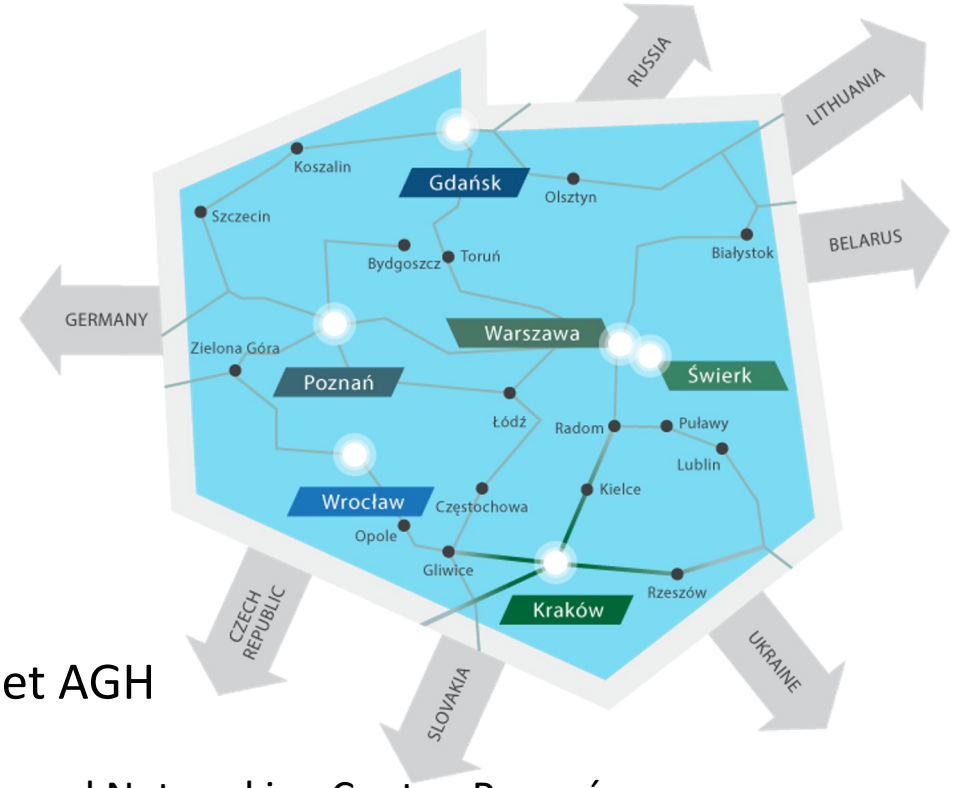
```
#!/bin/bash
#SBATCH --partition tutorial

## get tunneling info
XDG_RUNTIME_DIR=""
ipnport=$(shuf -i8000-9999 -n1)
ipnip=$(hostname -i)
user=$USER

module load jupyerlab

## start a cluster instance and launch Jupyter server
jupyter-notebook --no-browser --port=$ipnport --ip=$ipnip pyton-notebook.slurm
```

Jupyter notebooks

- User has to create a second tunnel from user's computer to login node of HPC resource (i.e. athena.cyfronet.pl)
  - `ssh -N -L <local-port>:<worker-node-ip>:<remote-port> username@athena.cyfronet.pl`
  - info about tunnel details `<local-port>`, `<worker-node-ip>`, `<remote-port>` are in log file of SLURM job
  - `username` – user's login
- After establishing both tunnels, Jupyter notebook is ready to start
  - open webpage `localhost:<local-port>` in browser on your local computer
  - remember about token, which is listed in a log file of SLURM job

PLGrid Infrastructure

- Projects:
  - PL-Grid
  - PLGrid Plus
  - PLGrid NG
  - PLGrid Core



- PLGrid Consortium
  - Coordinator: ACC Cyfronet AGH
  - Partners:
    - Poznan Supercomputing and Networking Center, Poznań
    - Interdisciplinary Centre for Mathematical and Computational Modelling, Warszawa
    - Wroclaw Centre for Networking and Supercomputing, Wrocław
    - Tricity Academic Computer Centre, Gdańsk
    - National Centre for Nuclear Research, Świerk

http://www.plgrid.pl/en/

PLGrid - computational infrastructure for science

- The PLGrid Infrastructure is available free of charge for Polish researchers and all those engaged in scientific activities in Poland
- On-line registration through PLGrid Users' Portal – https://portal.plgrid.pl
- User verification based on Polish Science Database – https://www.nauka-polska.pl

On PLGrid Users Portal user can

- apply for access to tools and services
- monitor utilization of resources
- manage their computational grants and grid certificates

Access to all PLGrid resources through **one account** and **one passphrase** (or grid certificate)

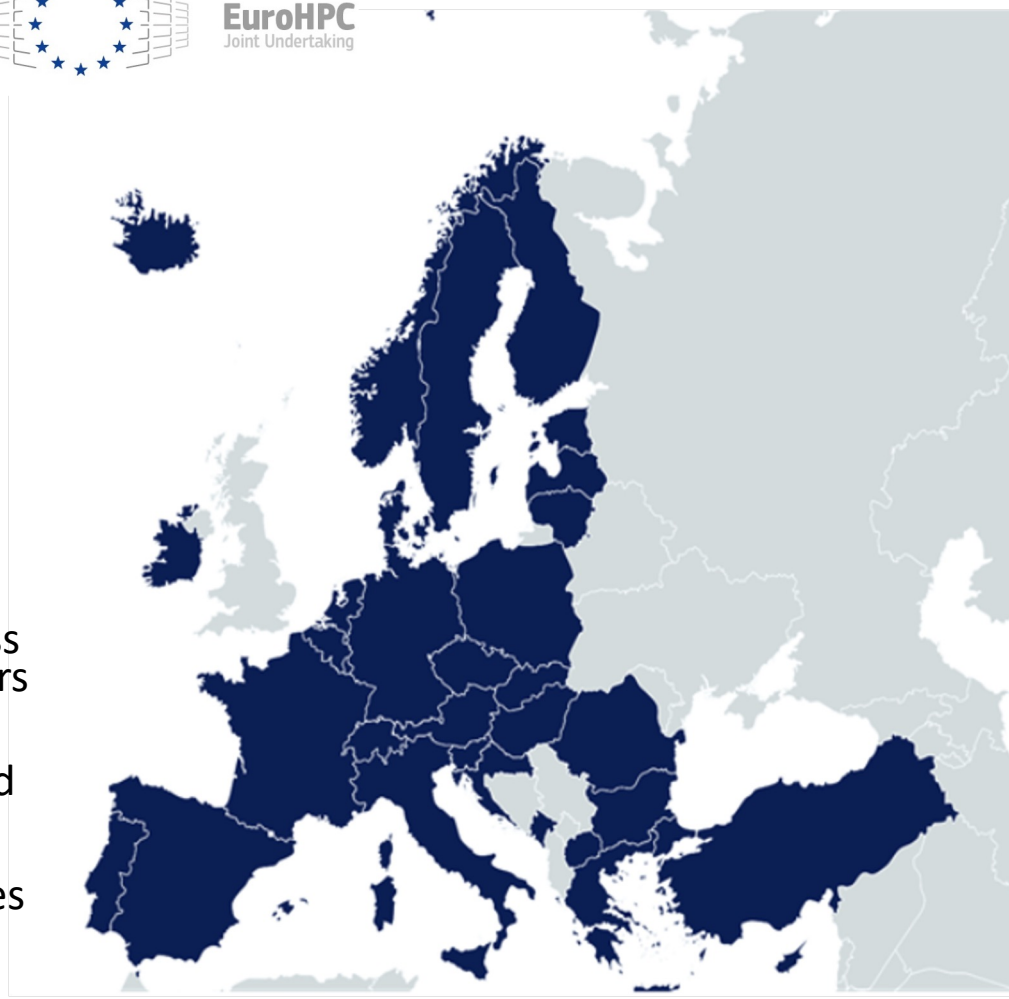
- The European High Performance Computing Joint Undertaking
  - 32 participating countries
  - the European Union (represented by the European Commission)
  - private partners

BDV BIG DATA VALUE ASSOCIATION

ETP 4 HPC EUROPEAN TECHNOLOGY PLATFORM FOR HIGH PERFORMANCE COMPUTING

- Goals
  - deploy top-of-the-range supercomputing infrastructures across Europe to support European HPC users wherever they are in Europe
  - implement an ambitious research and innovation agenda to develop a competitive HPC ecosystem and supply chain in Europe, which includes hardware, software, applications but also training and skills

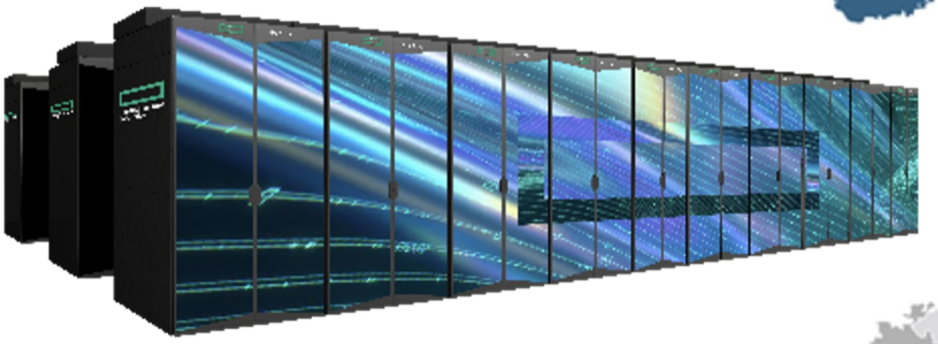
EuroHPC Joint Undertaking

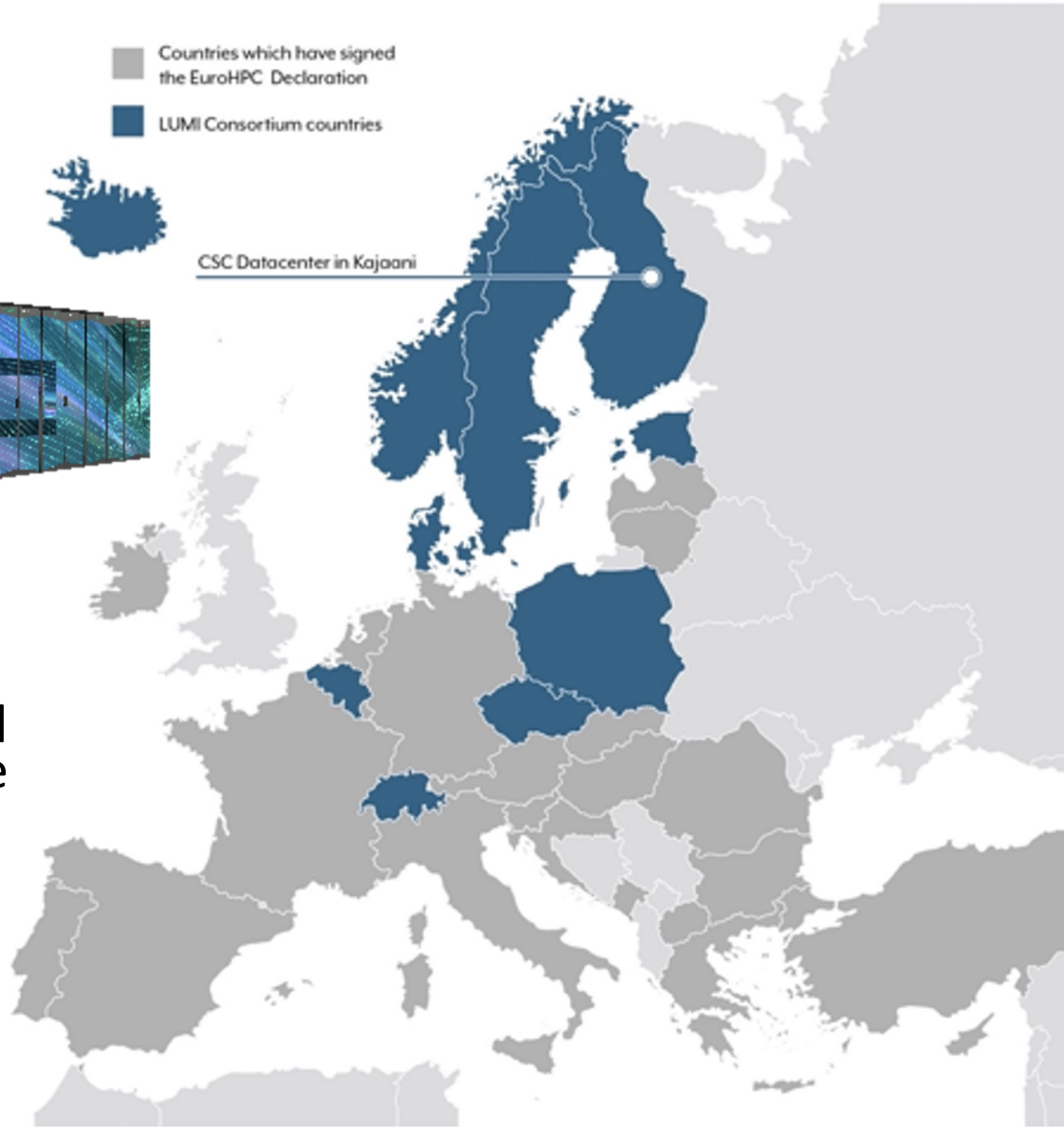


https://eurohpc-ju.europa.eu/

CYFRONET

LUMI





- LUMI will be an **HPE Cray EX** supercomputer manufactured by Hewlett Packard Enterprise
- Peak performance over 550 petaflop/s makes the system one of the world's fastest
- Available for users in
  - LUMI-C Q4 2021
  - LUMI-G Q1 2022

https://www.lumi-supercomputer.eu/

CYFRONET

- National Competence Centres for EuroHPC
- Goals
  - Establishing network of national HPC competence centers in all EuroHPC member states
  - Focus on cooperation between all stakeholders in european HPC
  - Training of scientific staff and development of HPC software in both academia and industrial environments

www.eurocc-project.eu

cc.eurohpc.pl

CYFRONET

AGH