



Parallel Programming (MPI) and Batch Usage (SLURM)

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Outline

- High Performance Computing (HPC)
 - TOP500
 - Architectures of HPC Systems
 - Message Passing Interface (MPI) Concepts
 - Collective functions
- Batch System
 - The Batch System Flow
- Practicals
 - Access the JURECA Cluster
 - Write and Submit a Batch Script

High Performance Computing

What is High Performance Computing?

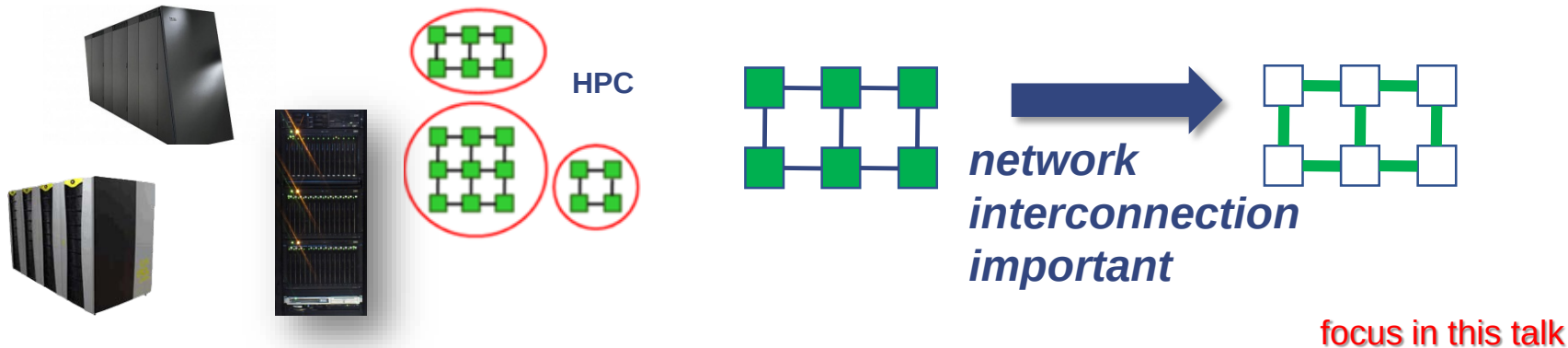
- **Wikipedia: ‘redirects from HPC to Supercomputer’**
 - A supercomputer is a computer at the frontline of contemporary processing capacity with particularly high speed of calculation
- **HPC includes work on ‘four basic building blocks’:**
 - **Theory** (numerical laws, physical models, speed-up performance, etc.)
 - **Technology** (multi-core, supercomputers, networks, storages, etc.)
 - **Architecture** (shared-memory, distributed-memory, interconnects, etc.)
 - **Software** (libraries, schedulers, monitoring, applications, etc.)

[1] Wikipedia ‘Supercomputer’ Online

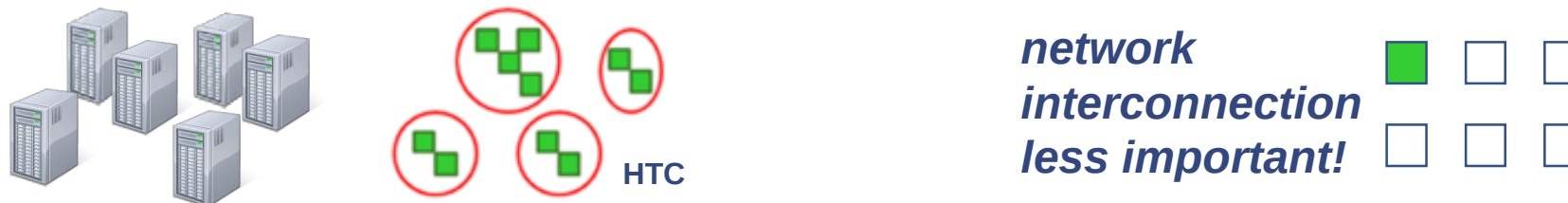
[2] Introduction to High Performance Computing for Scientists and Engineers

Understanding High Performance Computing

- **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



Parallel Computing

- All modern supercomputers heavily depend on parallelism
- We speak of parallel computing whenever a number of ‘compute elements’ (e.g. cores) solve a problem in a cooperative way

[2] Introduction to High Performance Computing for Scientists and Engineers

- ‘The measure of speed in **High Performance** Computing matters
 - Common measure for parallel computers established by **TOP500 list**
 - Based on **benchmark** for ranking the best 500 computers worldwide

[3] TOP 500 supercomputing sites

TOP 500 List (June 2018)

- Based on the **LINPACK** benchmark
- LINPACK** solves a dense system of linear equations of unspecified size. It covers only a single architectural aspect ('critics exist')

[4] *LINPACK Benchmark implementation*

- Alternatives realistic applications, benchmark suites and criteria exist

[5] *HPC Challenge Benchmark Suite*

[6] *JUBE Benchmark Suite*

[7] *The GREEN500*

Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	DOE/SC/Oak Ridge National Laboratory United States	Summit - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband IBM	2,282,544	122,300.0	187,659.3	8,806
2	National Supercomputing Center in Wuxi China	Sunway TaihuLight - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway NRCP	10,649,600	93,014.6	125,435.9	15,371
3	DOE/NNSA/LLNL United States	Sierra - IBM Power System S922LC, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband IBM	1,572,480	71,610.0	119,193.6	
4	National Super Computer Center in Guangzhou China	Tianhe-2A - TH-IVB-FEP Cluster, Intel Xeon E5-2692v2 12C 2.2GHz, TH Express-2, Matrix-2000 NUDT	4,981,760	61,444.5	100,678.7	18,482
5	National Institute of Advanced Industrial Science and Technology (AIST) Japan	AI Bridging Cloud Infrastructure (ABCI) - PRIMERGY CX2550 M4, Xeon Gold 6148 20C 2.4GHz, NVIDIA Tesla V100 SXM2, Infiniband EDR Fujitsu	391,680	19,880.0	32,576.6	1,649

.....

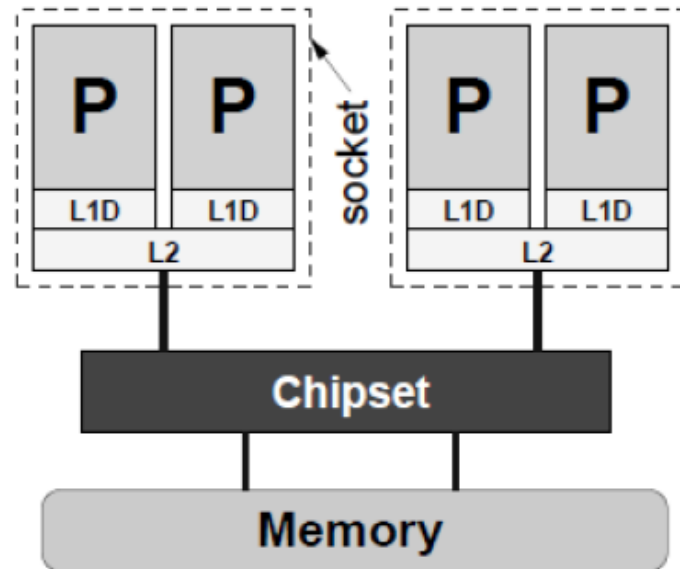
23	Forschungszentrum Juelich (FZJ) Germany	JUWELS Module 1 - Bull Sequana X1000, Xeon Platinum 8168 24C 2.7GHz, Mellanox EDR InfiniBand/ParTec ParaStation ClusterSuite Bull, Atos Group	114,480	6,177.7	9,891.1	1,361
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Architectures of HPC Systems

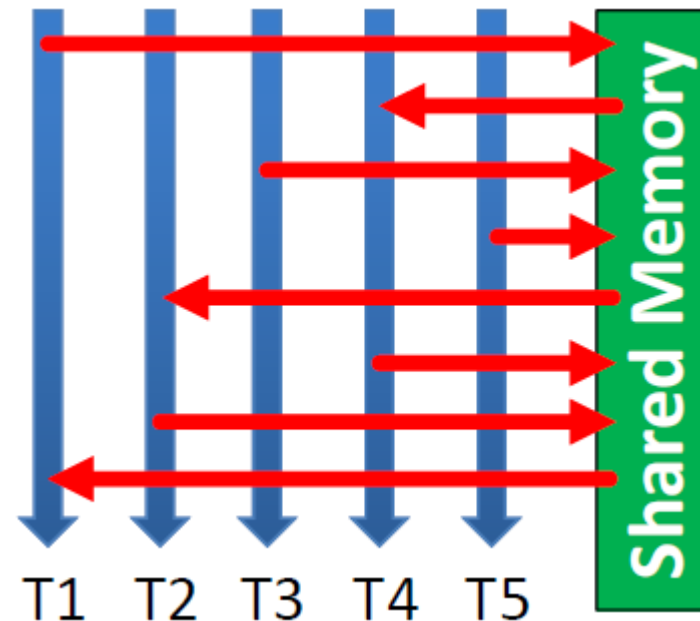
- Two dominant types of architectures
 - **Shared-Memory Computers**
 - **Distributed-Memory Computers**
- Often hierarchical (hybrid) systems of both in practice
- More recently both above are considered as '**programming models**'
 - **Shared-Memory** parallelization with **OpenMP**
 - **Distributed-Memory** parallel programming with **MPI**

Shared-Memory Computers

- System where a number of CPUs work on a common, shared physical address space
- Programming using **OpenMP** (set of compiler directives to 'mark parallel regions')
- Enables immediate access to all data by all processors without explicit communication



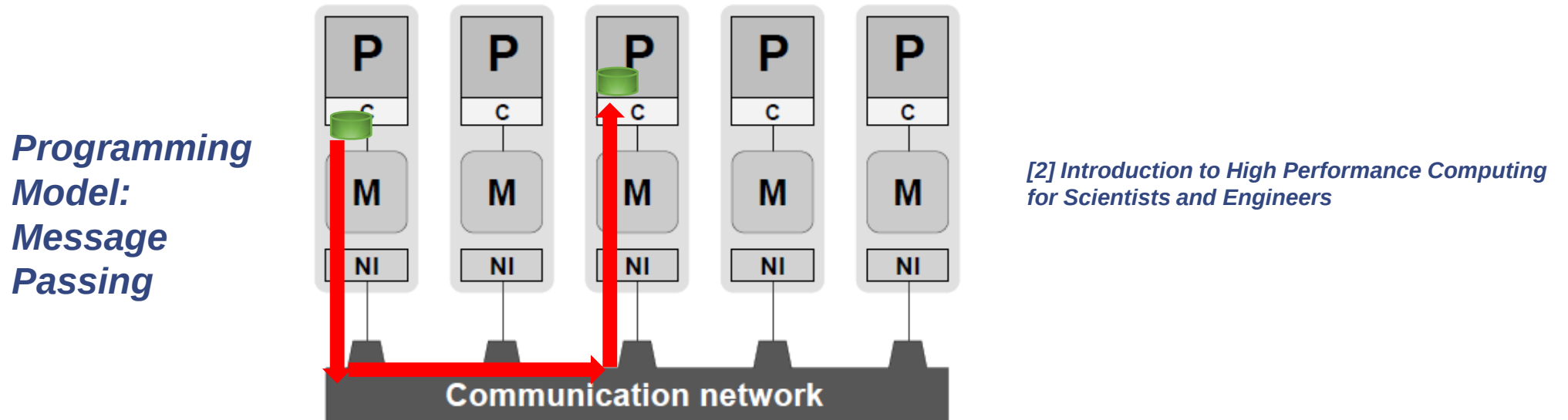
[2] Introduction to High Performance Computing for Scientists and Engineers



[8] OpenMP API Specification

Distributed-Memory Computers

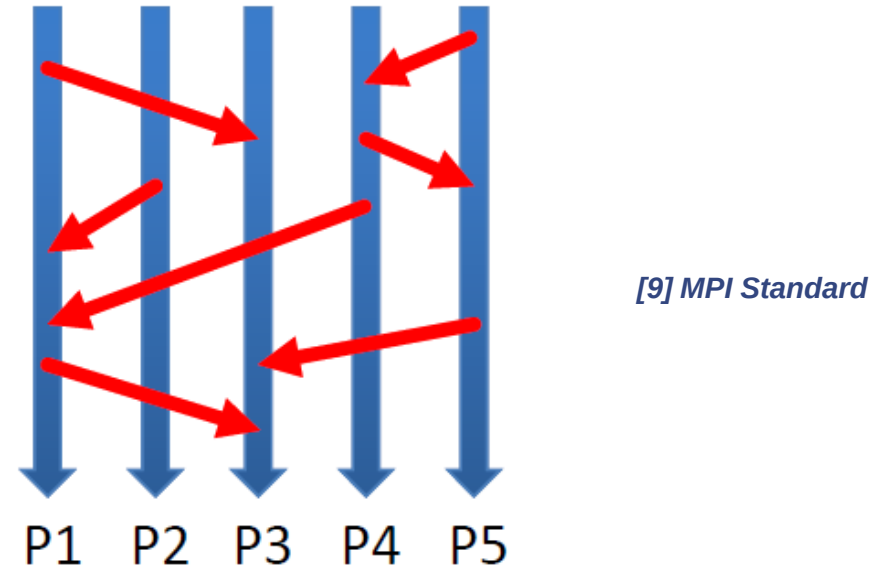
- Establishes a 'system view' where no process can access another process' memory directly



- Processors communicate via Network Interfaces (NI)
- NI mediates the connection to a Communication network
- This setup is rarely used -> a programming model view today

Programming with Distributed Memory using MPI

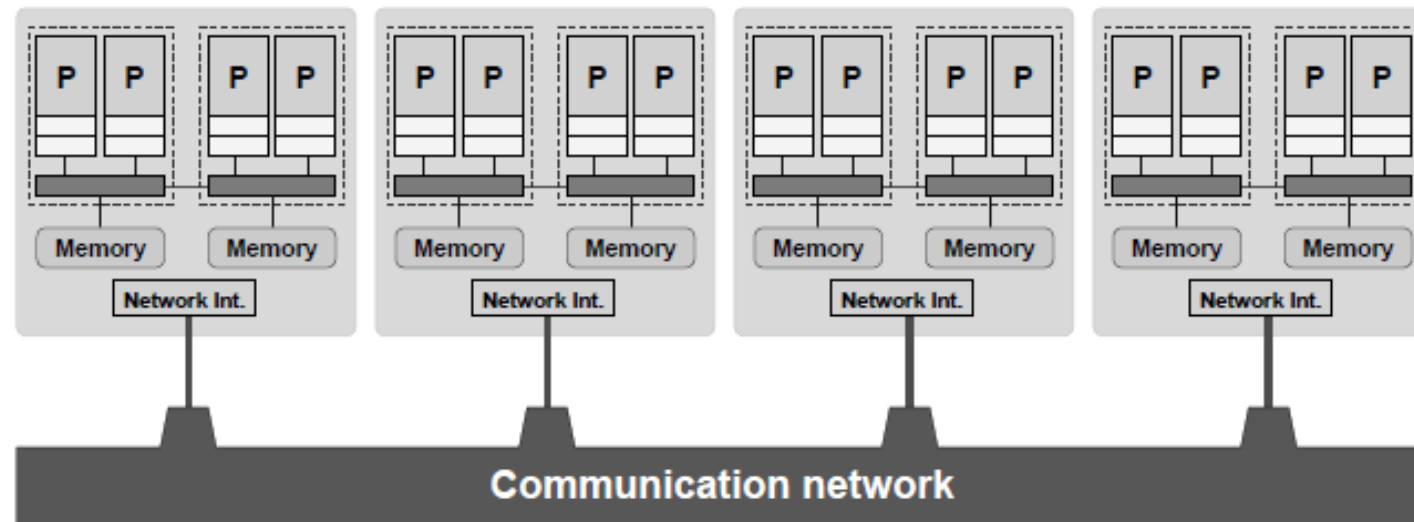
- Enables explicit message passing as communication between processors



- No **remote memory access** on distributed-memory systems
- Require to '**send messages**' back and forth between processes PX
- Programming is tedious & complicated, but **most flexible method**

Hierarchical Hybrid Computers

- Mixture of shared-memory and distributed-memory systems
- Nowadays large-scale ‘hybrid’ parallel computers have shared-memory building blocks interconnected with a fast network (e.g., InfiniBand)



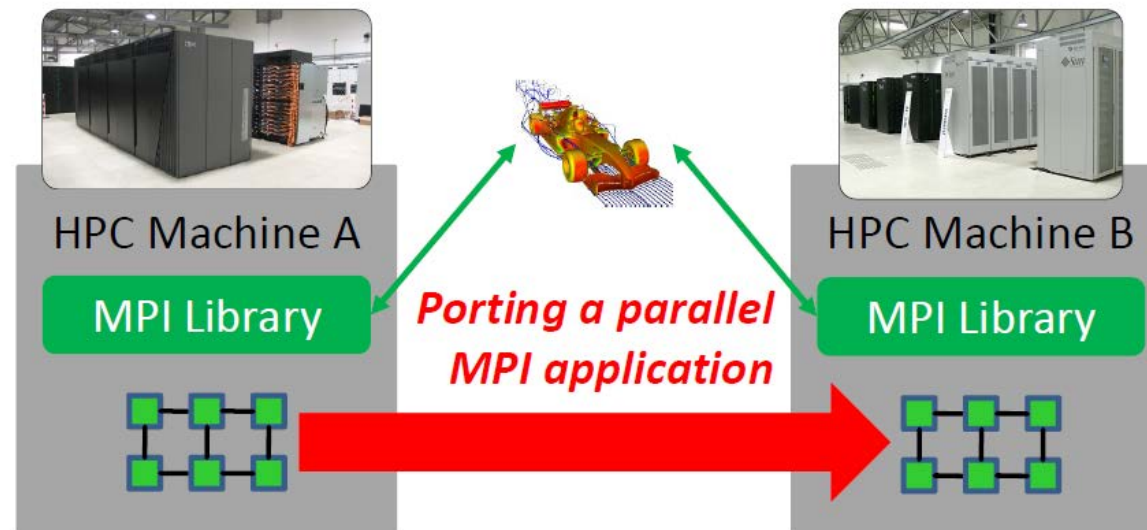
What is Message Passing Interface (MPI)?

- **‘Communication library’** abstracting from low-level network view
 - Offers 500+ available functions to communicate between computing nodes
 - Practice reveals: parallel applications often require just ~12 (!) functions
 - Includes routines for efficient ‘parallel I/O’ (using underlying hardware)
- Supports **‘different ways of communication’**
 - ‘Point-to-point communication’ between two computing nodes ($P \leftrightarrow P$)
 - Collective functions involve ‘N computing nodes in useful communication’
- Deployment on Supercomputers
 - Installed on (almost) all parallel computers
 - Different languages: C, Fortran, Python, R, etc.
 - Careful: different versions exist

Recall ‘computing nodes’ are independent computing processors (that may also have N cores each) and that are all part of one big parallel computer

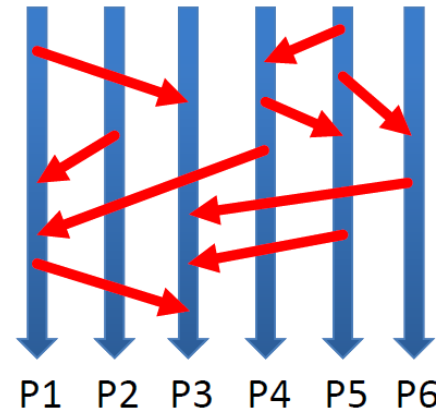
Key Features of MPI

- Simplify programming in parallel programming, **focus on applications**
- It is not designed to handle any communication in computer networks
- Designed for performance within large parallel computers (e.g. no security)
- Several open-source well-tested implementations of MPI
- It enables portability of parallel applications

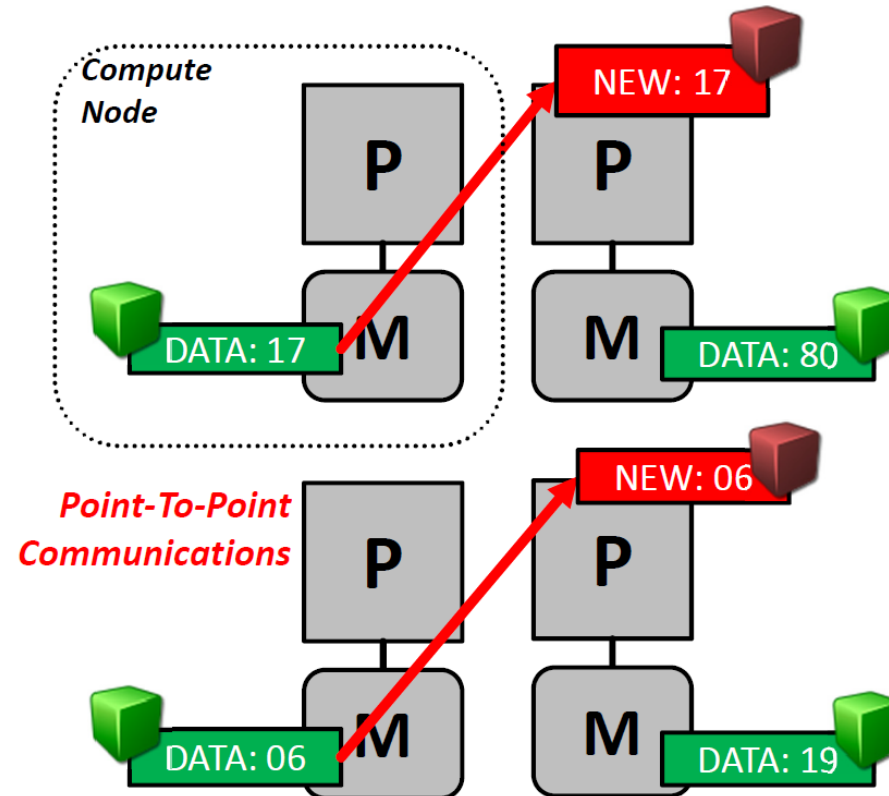
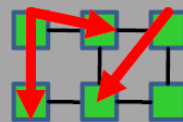


Message Passing: Exchanging Data

- Each processor has its own data and memory that cannot be accessed by other processors

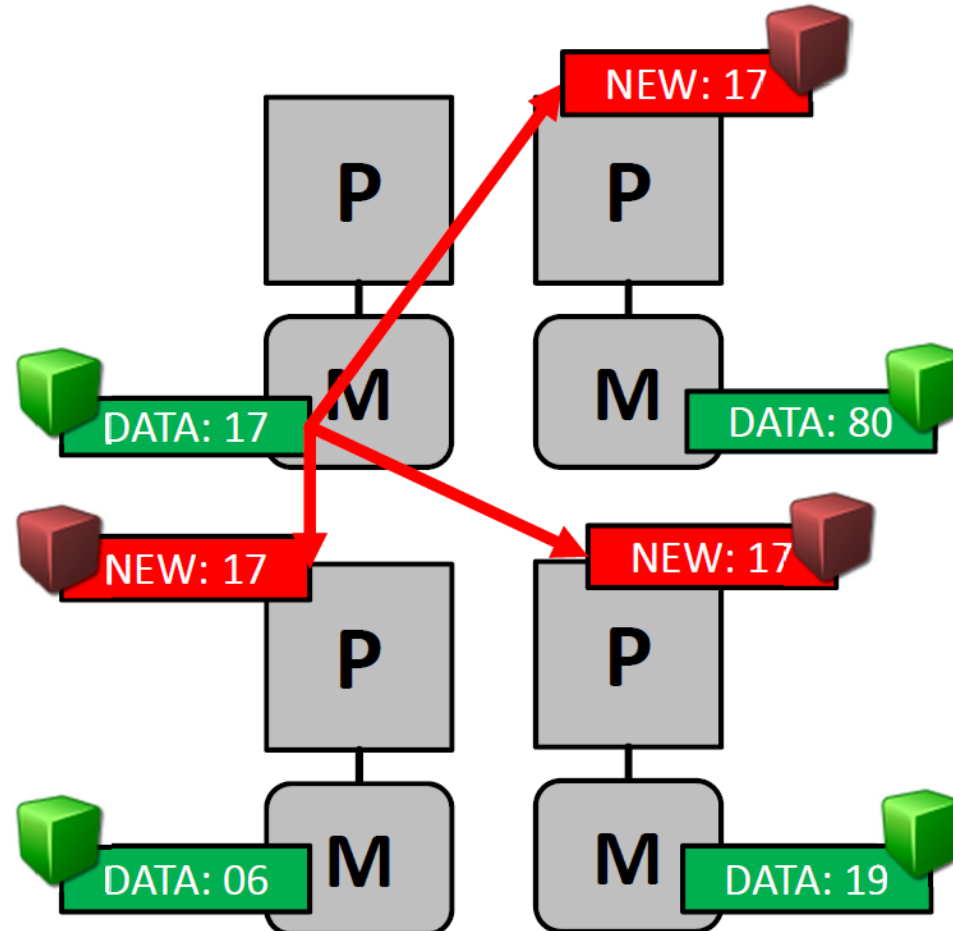


HPC Machine



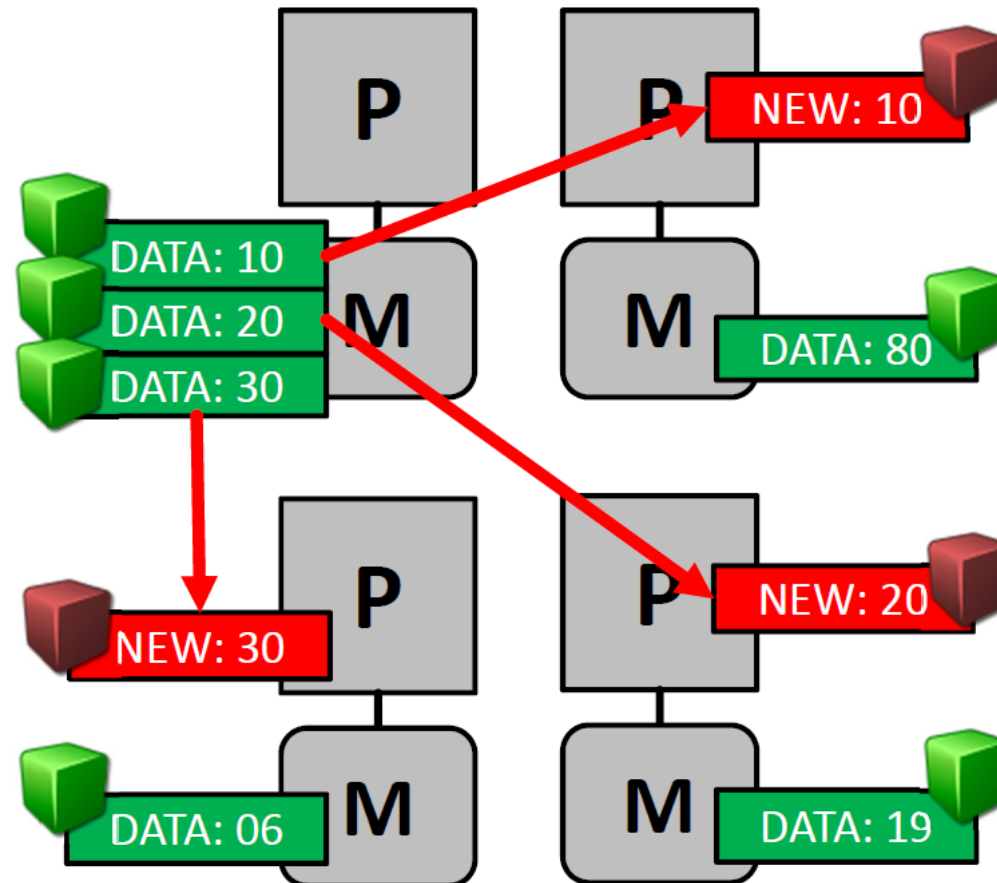
Collective Functions: Broadcast (one-to-many)

- Broadcast distributes the **same** data to many or even all other processors



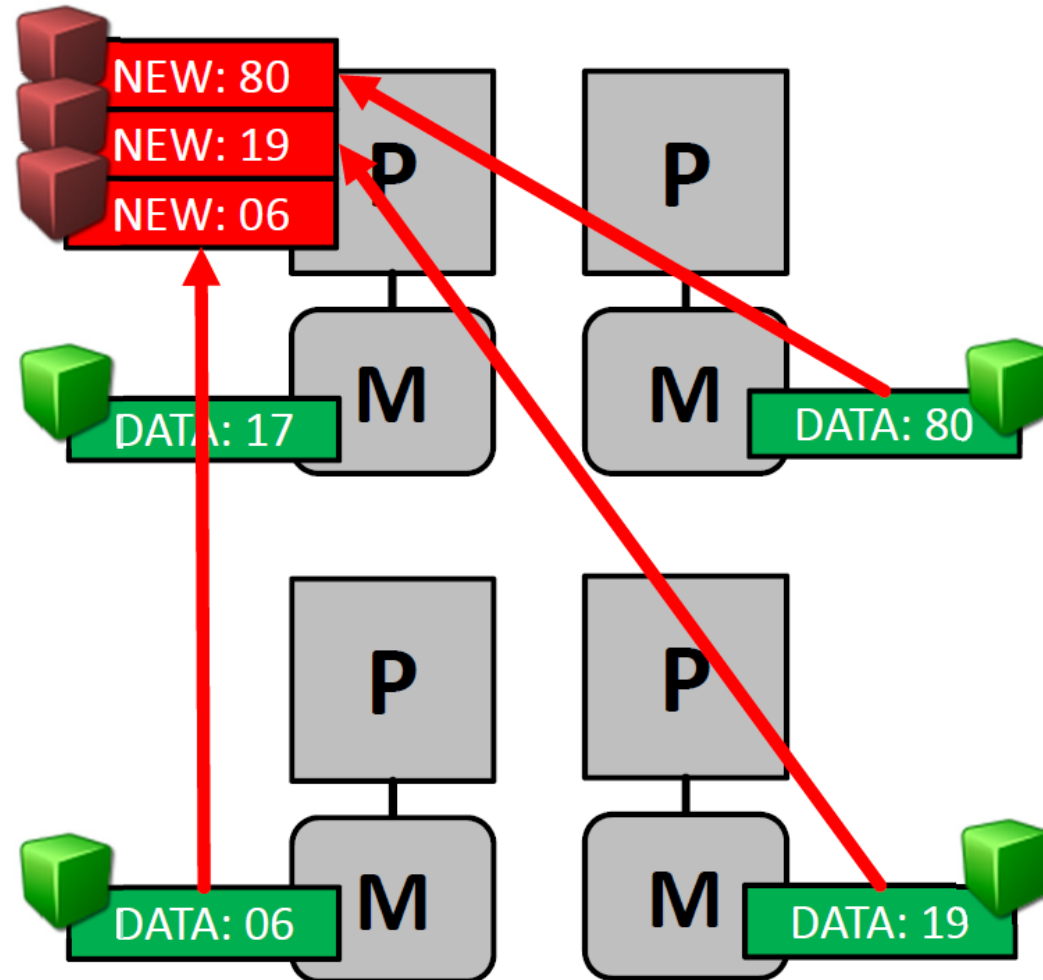
Collective Functions: Scatter (one-to-many)

- Scatter distributes **different** data to many or even all other processors



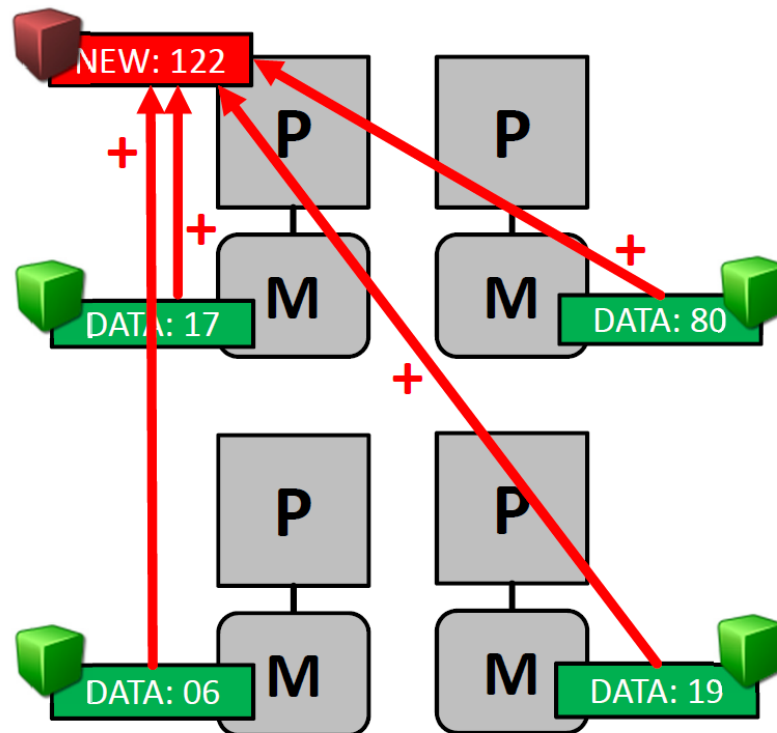
Collective Functions: Gather (many-to-one)

- Gather **collects** data from many or even all other processors to one specific processor



Collective Functions: Reduce (many-to-one)

- Each Reduce combines collection with computation based on data from many or even all other processors
- Usage of reduce includes finding a **global minimum or maximum, sum, or product** of the different data located at different processors



+ global sum as example

Batch System

What is a Batch System?

- Mechanism to control access by many users to shared computing resources
- Queuing / scheduling system for the jobs of the users
- Manages the reservation of resources and job execution
- Allows users to “fire and forget”, long calculations or many jobs (“production runs”)

Why do we need a Batch System?

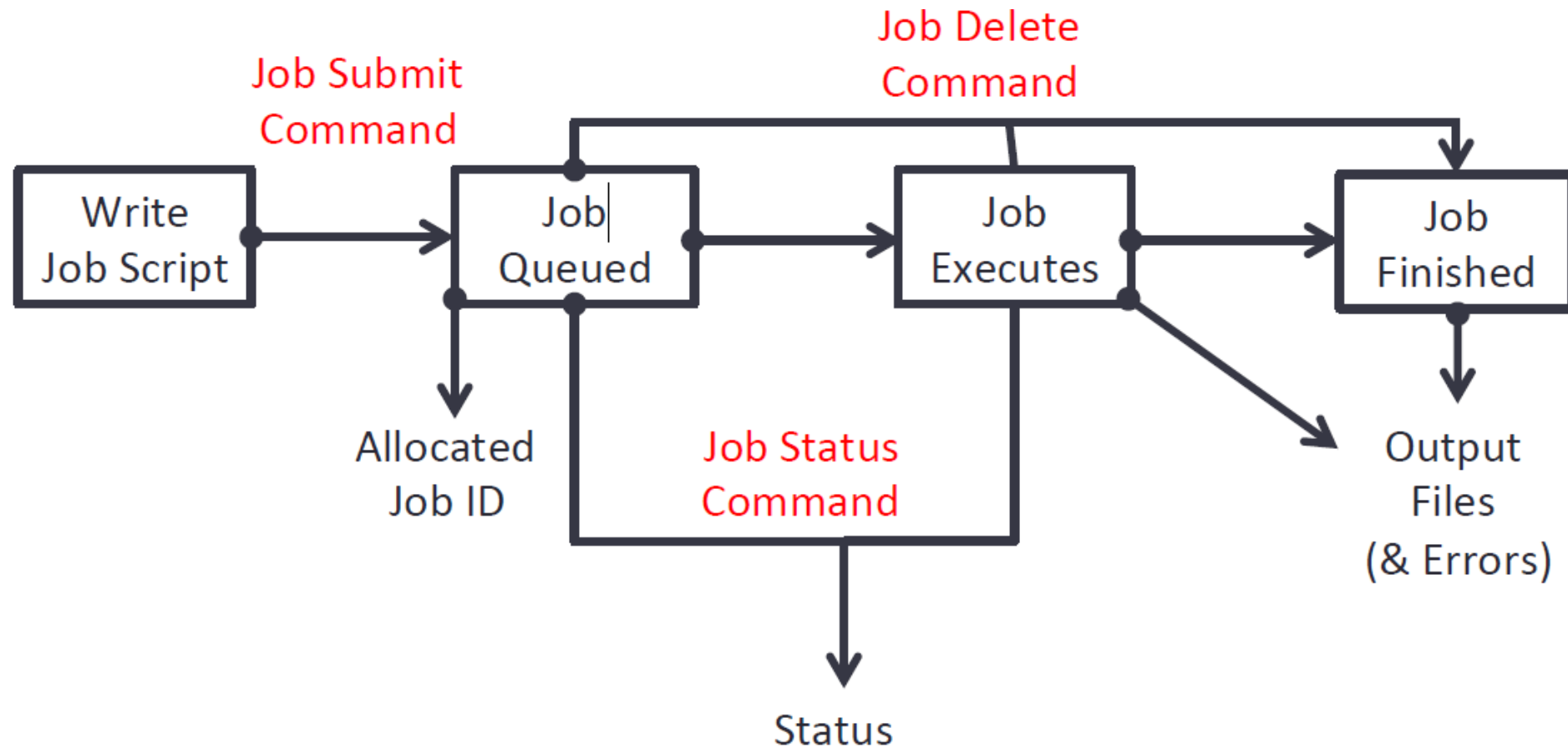
- Opposite of interactive processing
- Ensure all users get a fair share of compute resources (demand usually exceeds supply)
- To ensure the machine is utilized as efficiently as possible
- To track usage - for accounting and budget control
- To mediate access to other resources e.g. software licences

The only access to significant resources on the HPC machines is through the batch process

How to use a Batch System

1. Setup a job, consisting of:
 - Commands that run one or more calculations / simulations
 - Specification of compute resources needed to do this
2. Submit your job to the batch system
 - Job is placed in a queue by the scheduler
 - Will be executed when there is space and time on the machine
 - Job runs until it finishes successfully, is terminated due to errors, or exceeds a time limit
3. Examine outputs and any error messages

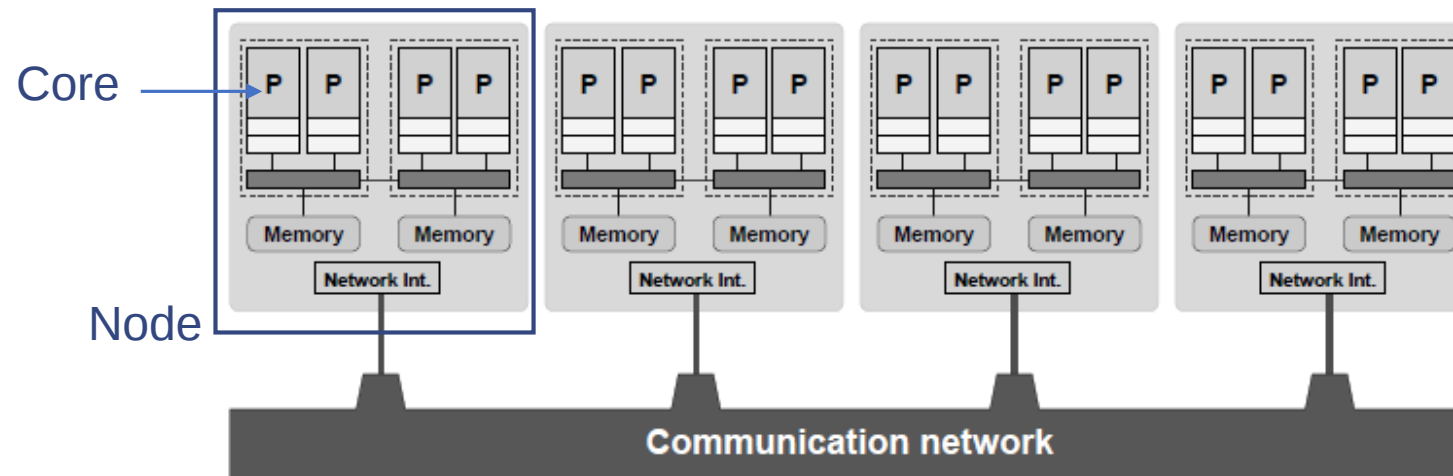
Batch System Flow



[11] Batch Systems

JSC Batch Model

- **Slurm** is the chosen Batch System (Workload Manager) for JURECA
 - **Scheduling according to priorities:** jobs with the highest priorities will be scheduled next
 - **Backfilling scheduling algorithm:** the scheduler checks the queue and may schedule jobs with lower priorities that can fit in the gap created by freeing resources for the next highest priority jobs
 - **No node-sharing:** the smallest allocation for jobs is one compute node. Running jobs do not disturb each other.
 - $\text{Accounted CPU-Quotas/job} = \text{Number-of-nodes} \times \text{Walltime} \times \text{cores/node}$



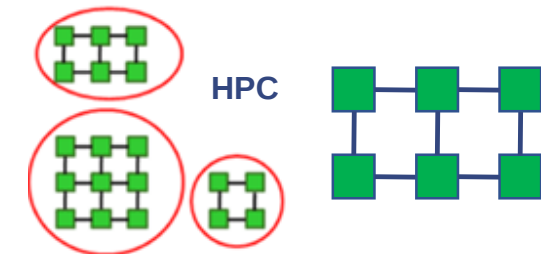
Practicals

JURECA HPC System at JSC

- Characteristics
 - Login nodes with 256 GB memory per node
 - 45,216 CPU cores
 - 1.8 (CPU) + 0.44 (GPU) Petaflop/s peak performance
 - **Two Intel Xeon E5-2680 v3 Haswell CPUs per node: 2 x 12 cores, 2.5 GHz**
 - 75 compute nodes equipped with two NVIDIA K80 GPUs (2 x 4992 CUDA cores)
- Architecture & Network
 - Based on T-Platforms V-class server architecture
 - Mellanox EDR InfiniBand high-speed network with non-blocking fat tree topology
 - 100 GiB per second storage connection to JUST



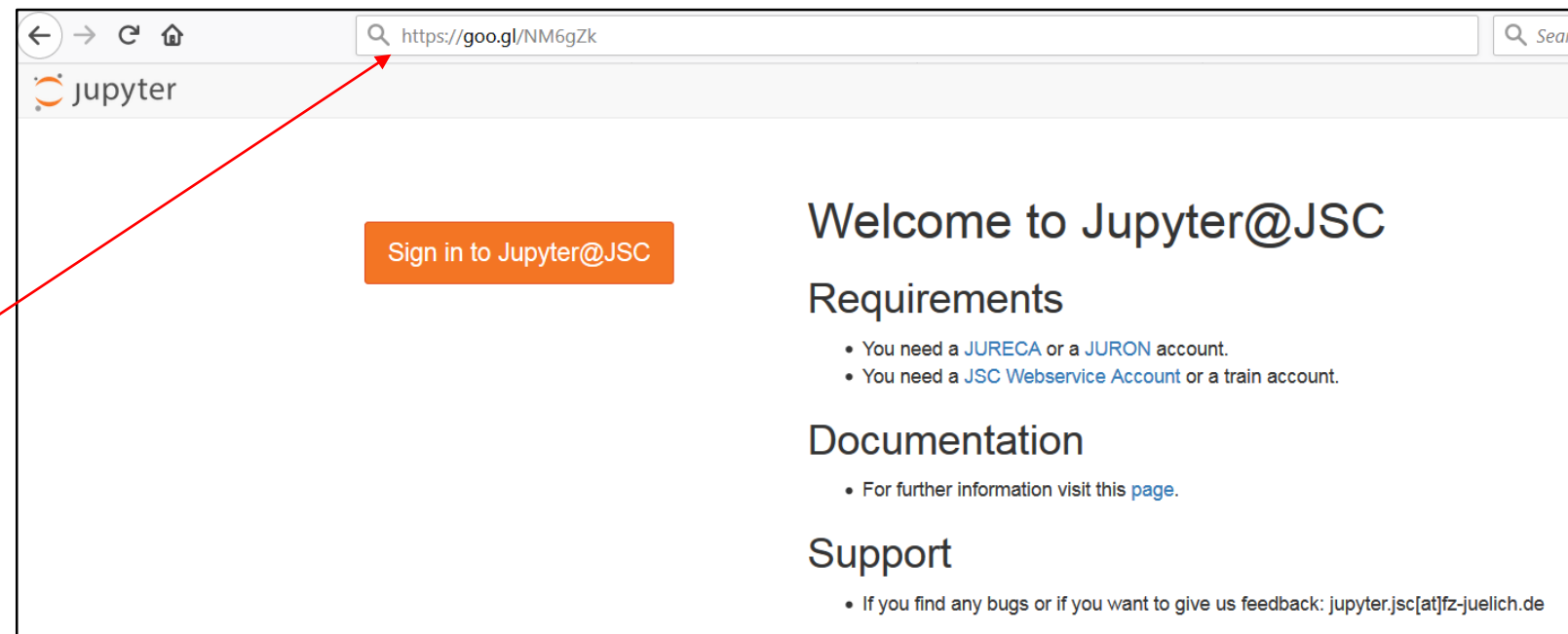
[10] JURECA HPC System



Access JURECA Cluster (Step 1)

- Open your web browser
- Connect to <https://goo.gl/NM6gZk>
- Click on the orange button “Sign in to Jupyter@JSC”

Username: train0??
SSH Passphrase: ??????????
Login here: <https://goo.gl/NM6gZk>
<https://igarss2018.org/Tutorials.asp#FD-4>



Access JURECA Cluster (Step 2)

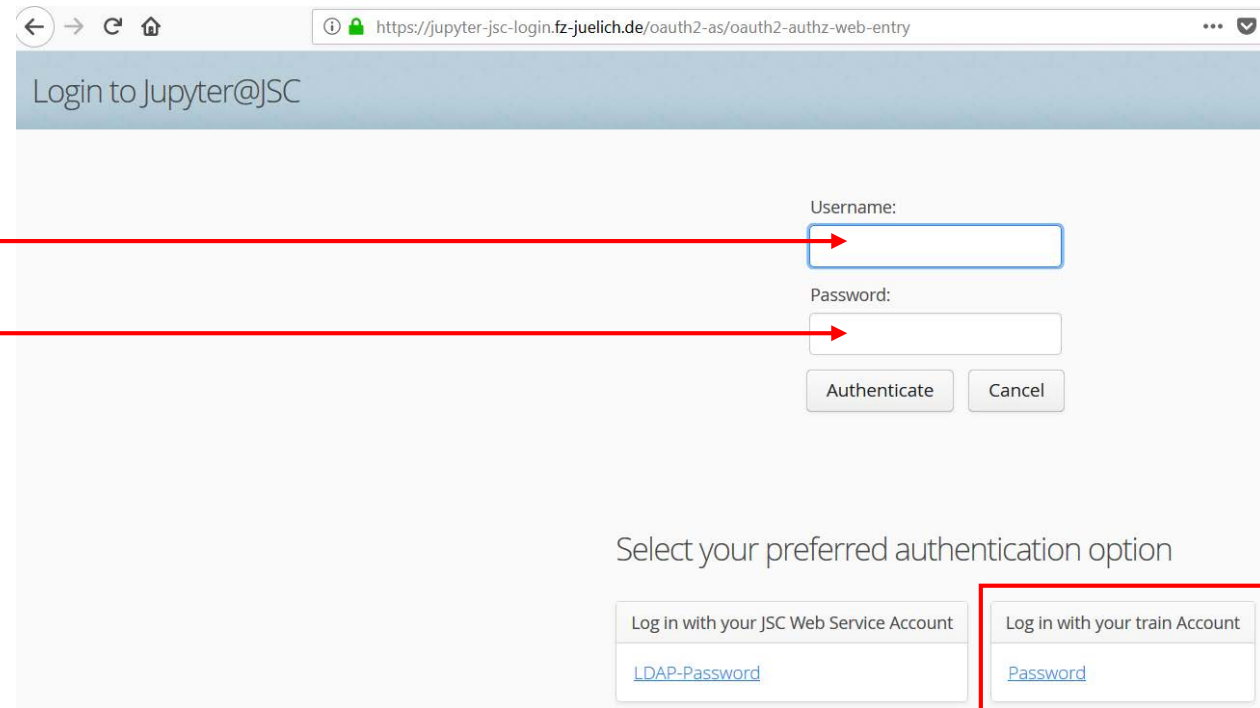
- Select authentication option: **“Password”** (Log in your train Account)
- Insert Username and SSH Passphrase
- Authenticate

Username: train0??

SSH Passphrase: ??????????

Login here: <https://goo.gl/NM6gZk>

<https://igarss2018.org/Tutorials.asp#FD-4>

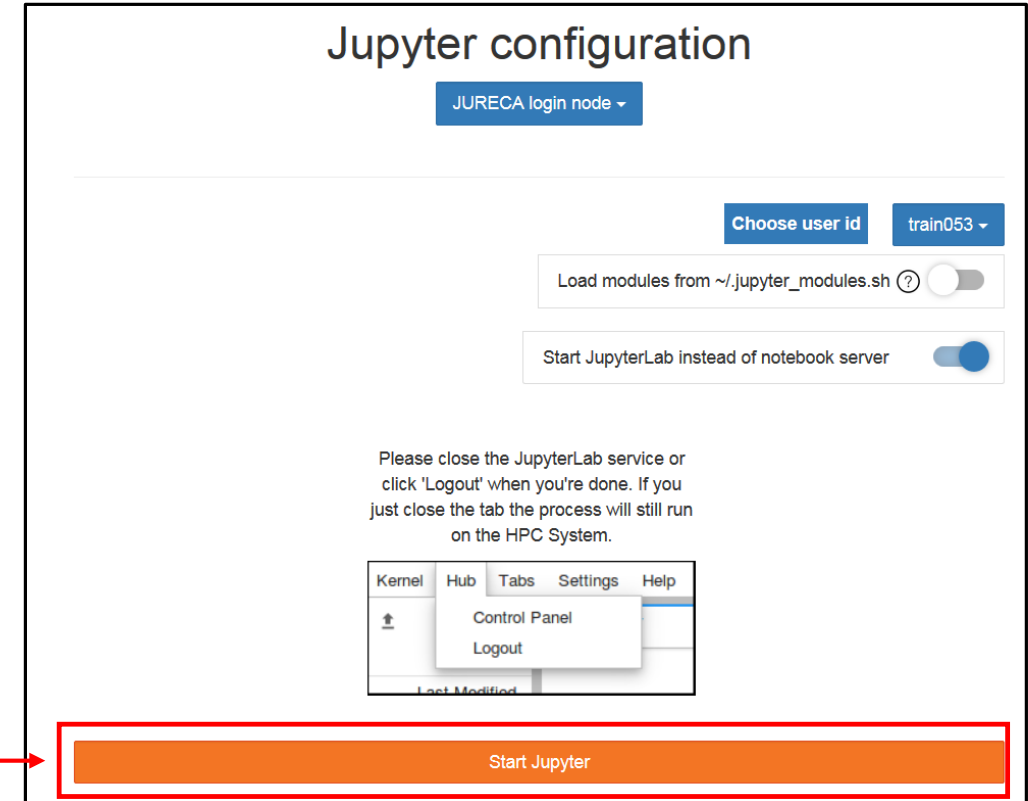


Access JURECA Cluster (Step 3)

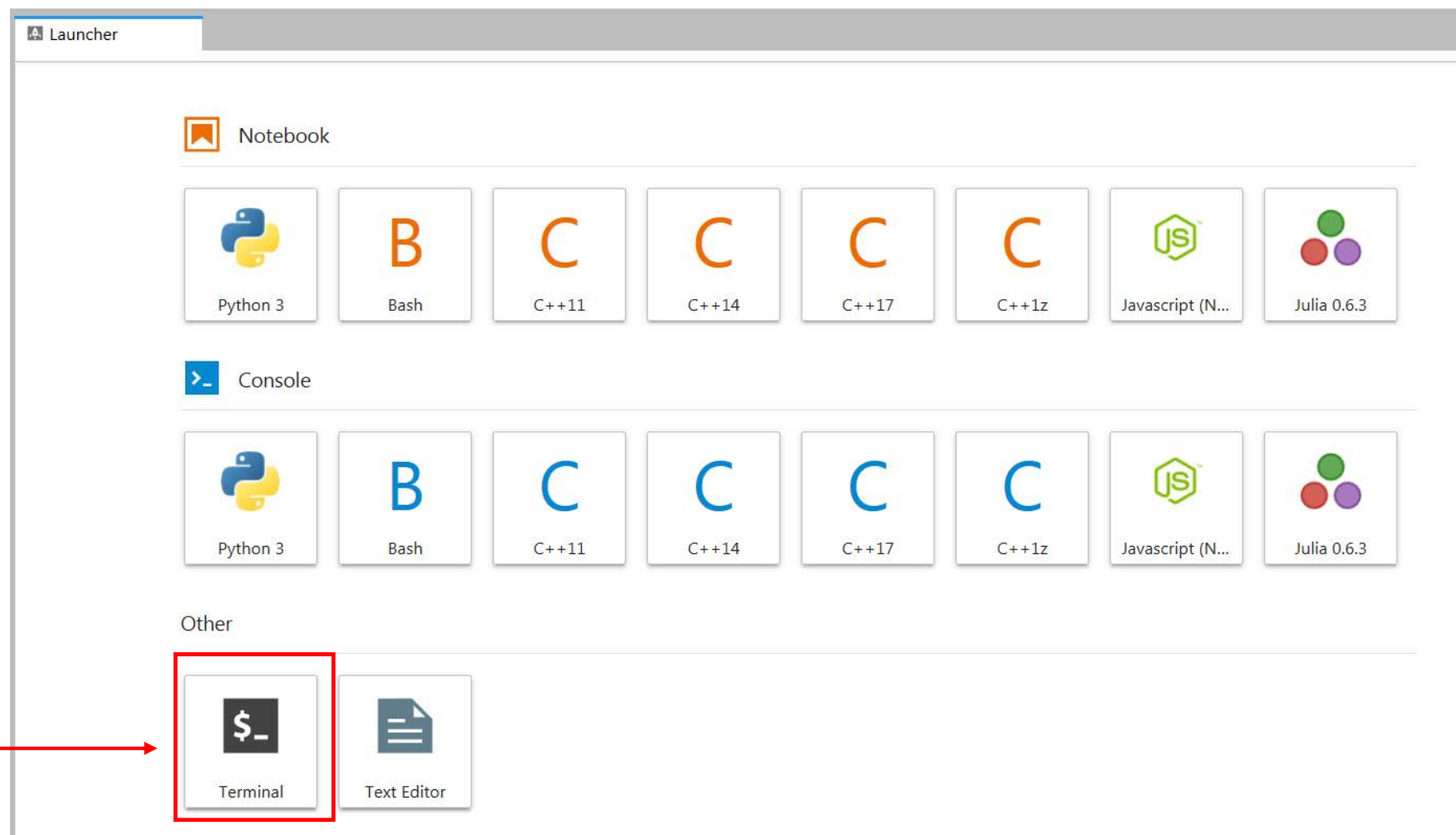
- Click on



- Click on



Access JURECA Cluster (Step 4)



- Click on

JURECA Cluster Accessed

```
train053@jrl05: X
*
* Information about the system, latest changes, user documentation and FAQs:
* http://www.fz-juelich.de/ias/jsc/jureca
*
*****
* ### Known Issues ###
*
* An up-to-date list of known issues on the system is maintained at
* http://www.fz-juelich.de/ias/jsc/jureca-known-issues
*
* Open issues:
* - Intel compiler error with std::valarray and
*   optimized headers, added 2016-03-20
*
* 2018-04-25
*****
* ### File system performance during extension of JUST cluster ###
*
* In the following weeks data will be migrated from JUST4 to JUST5. During
* this time I/O performance might be impaired. We try to keep the effect on
* user applications as low as possible.
*
* Thank you for your understanding.
*
* 2018-04-25
*****
* ### Offline maintenance ###
*
* Booster Module will be unavailable for software and hardware maintenance on
* - Thursday, 2018-07-12 between 08:30 and 18:30
*
* JURECA will be unavailable for software and hardware maintenance on
* - Tuesday, 2018-07-31 between 08:30 and 18:30
*
* 2018-07-05
*****
* ### Restricted access to $ARCH ###
*
* Access to $ARCH may be limited due to Problems with one of our tape
* libraries. We apologize for the inconvenience caused.
*
* 2018-07-06
*****
[train053@jrl05 ~]$
```

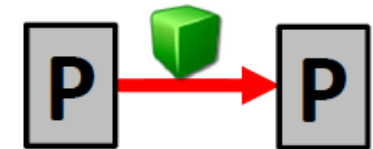
Navigate to the Material

- **ls** command: it shows the files and directories that are present in your current location
- The material of the tutorial is inside the **igarss_tutorial** folder
- **cd** command: use to access a folder (do **\$ cd igarss_tutorial**)
- The material of this first lecture is in the **mpi_hello_world** folder (do **\$ cd mpi_hello_world**)

```
[train053@jrl06 ~]$ ls
bin  igarss_tutorial
[train053@jrl06 ~]$ cd igarss_tutorial/
[train053@jrl06 igarss_tutorial]$ ls
3dcnn  mpi_hello_world  psvm
[train053@jrl06 igarss_tutorial]$ cd mpi_hello_world/
[train053@jrl06 mpi_hello_world]$ ls
hello_world  hello_world.c
[train053@jrl06 mpi_hello_world]$
```

Start 'Thinking' Parallel

- **Parallel MPI programs know about the existence of other processes of it** and what their own role is in the bigger picture
- MPI programs are written in a **sequential** programming language, but **executed in parallel**
 - Same MPI program runs on all processes (**Single Program Multiple Data**)
- **Data exchange** is key for design of applications
 - Sending/receiving data **at specific times** in the program
 - **No shared memory** for sharing variables with other remote processes
 - Messages can be **simple variables** (e.g. a word) or **complex structures**
- Start with the **basic building blocks** using MPI
 - Building up the '**parallel computing environment**'



```
int main(int argc, char** argv) {  
  
    return 0;  
}
```

- Normally the 'return code' denotes whether the program exit was ok (0) or problematic (-1)

- ```
[train053@jrl06 mpi_hello_world]$ ls
hello_world hello_world.c
```

# (MPI) Basic Building Blocks: Variables & Output

*'standard C programming...'*

```
#include <stdio.h>

int main(int argc, char** argv) {
 int rank, size;

 printf("Hello World, I am %d of %d\n", rank, size);

 return 0;
}
```

- Libraries can be used by including C header files, here library for screen outputs for example

- Two integer variables that are later useful for working with specific data obtained from MPI library

- Output with printf using stdio library: 'Hello World' and which process is printing out of the summary of all n processes

```
[train053@jrl06 mpi_hello_world]$ ls
hello_world hello_world.c
```

# MPI Basic Building Blocks: Header & Init/Finalize

*'standard C programming including MPI library use...'*

```
#include <stdio.h>
#include <mpi.h>

int main(int argc, char** argv) {
 int rank, size;

 MPI_Init(&argc, &argv);

 printf("Hello World, I am %d of %d\n", rank, size);

 MPI_Finalize();
 return 0;
}
```

- Libraries can be used by including C header files, here library for MPI included

- The MPI\_INIT() function initializes the MPI environment and can take inputs via the main() function arguments

- MPI\_Finalize() shuts down the MPI environment (after this statement no parallel execution of the code can take place)

```
[train053@jrl06 mpi_hello_world]$ ls
hello_world hello_world.c
```

# MPI Basic Building Blocks: Rank & Size Variables

*'standard C programming including MPI library use...'*

```
#include <stdio.h>
#include <mpi.h>

int main(int argc, char** argv) {
 int rank, size;

 MPI_Init(&argc, &argv);
 MPI_Comm_size(MPI_COMM_WORLD, &size);
 MPI_Comm_rank(MPI_COMM_WORLD, &rank);

 printf("Hello World, I am %d of %d\n", rank, size);

 MPI_Finalize();
 return 0;
}
```

- **MPI\_COMM\_WORLD** communicator constant denotes the 'region of communication', here all processes

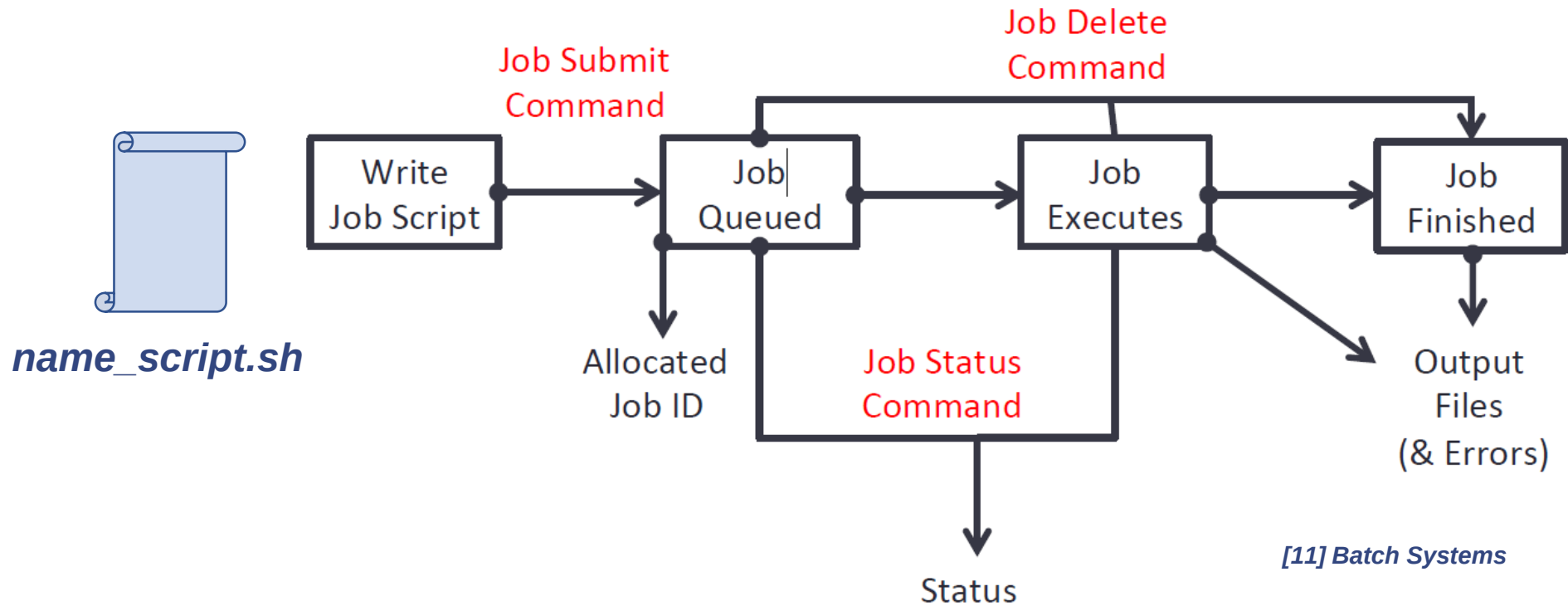
- The **MPI\_Comm\_size()** function determines the overall number of *n* processes in the parallel program: stores it in variable *size*

- The **MPI\_Comm\_rank()** function determines the unique identifier for each processor: stores it in variable *rank* with values (0 ... *n*-1)

```
[train053@jrl06 mpi_hello_world]$ ls
hello_world hello_world.c
```

# Job Script

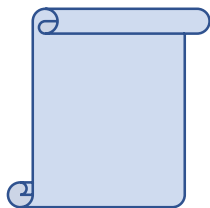
- Text file containing
  - Job setup information for the batch system
  - Commands to be executed



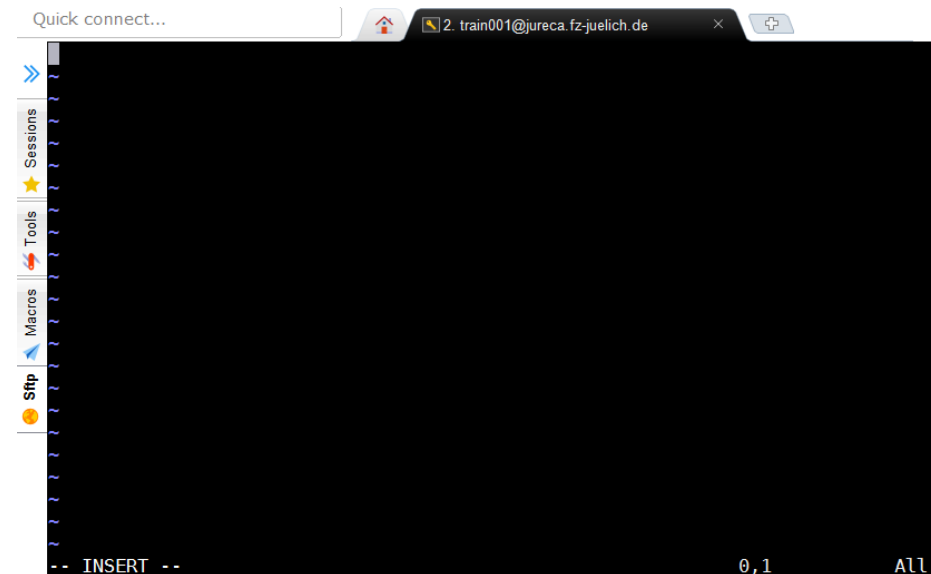
[11] Batch Systems

# Job Script - File Creation with vi

- **vi** (visual editor): is the default editor that comes with the UNIX operating system
- It has two modes of operation:
  - **Command mode** commands: cause action to be taken on the file
  - **Insert mode**: entered text is inserted into the file
- Do the following steps:
  - **\$ vi submit\_hello\_world.sh**
  - **Press i on your keyboard**

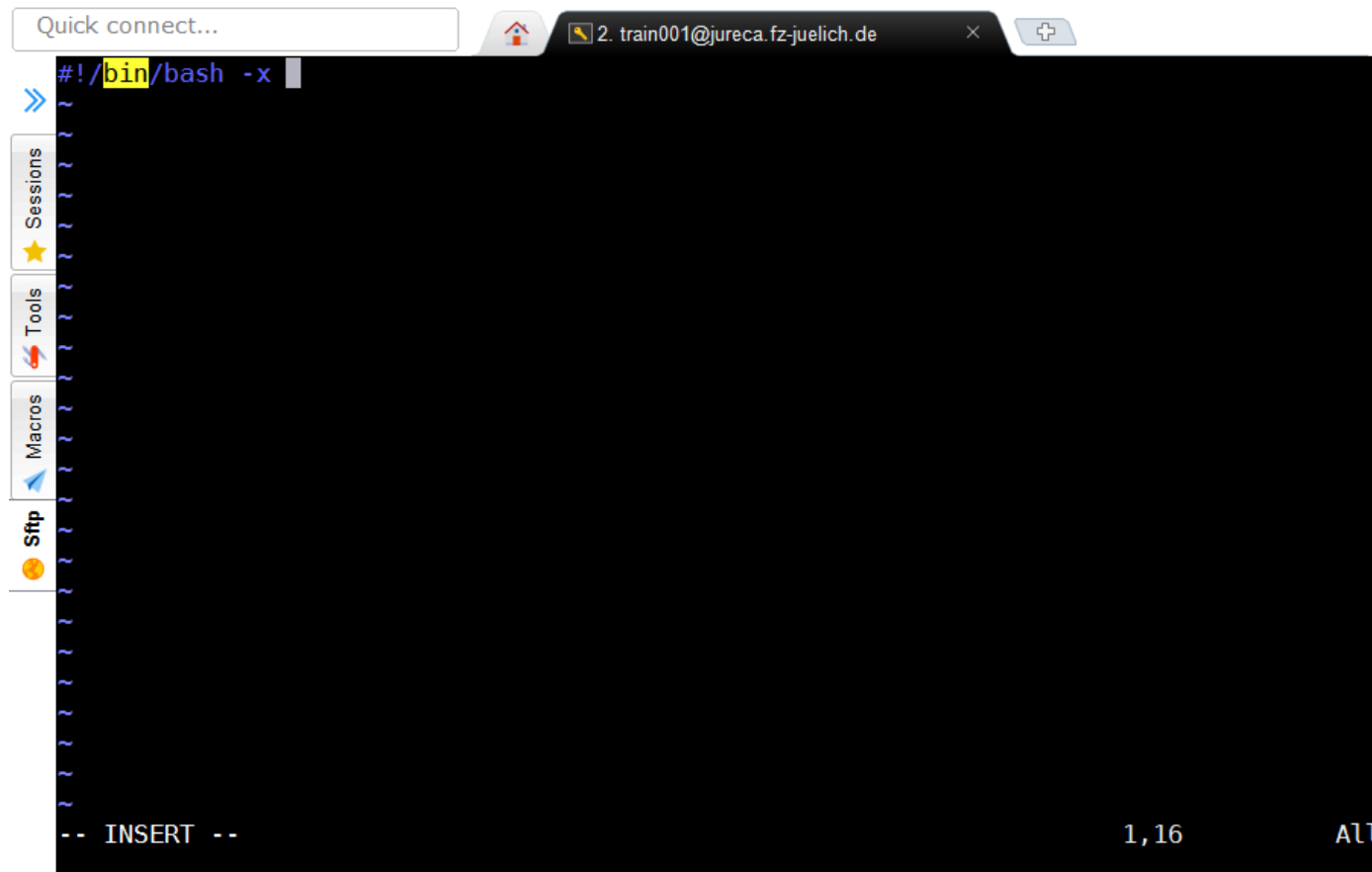


```
[train053@jrl06 mpi_hello_world]$ vi submit_hello_world.sh
```



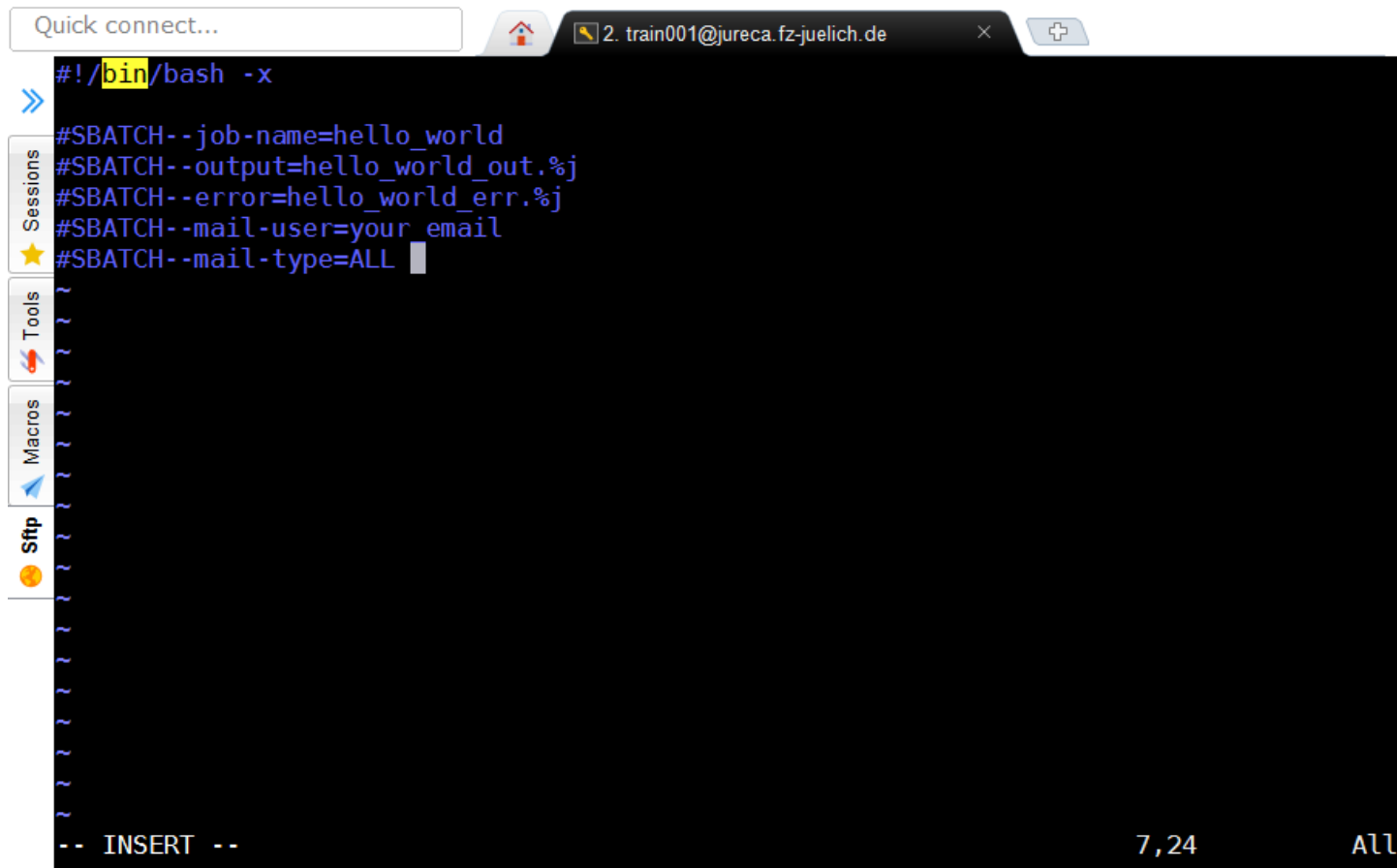
# Job Script Editing (1)

- Start the script with the shebang (i.e., absolute path to the bash interpreter)
- **Type as a first line of your script: `#!/bin/bash -x`** (execute the file using the bash shell)



The screenshot shows a code editor window with a dark background. The top bar displays a search field labeled "Quick connect..." and a tab titled "2. train001@jureca.fz-juelich.de". The main editing area contains the text `#!/bin/bash -x`, where `bin` is highlighted in yellow. On the left side, there is a vertical sidebar with icons for "Sessions", "Tools", "Macros", and "Sftp". At the bottom of the editor, the status bar shows "-- INSERT --" on the left, "1,16" in the center, and "All" on the right.

# Job Script Editing (2)

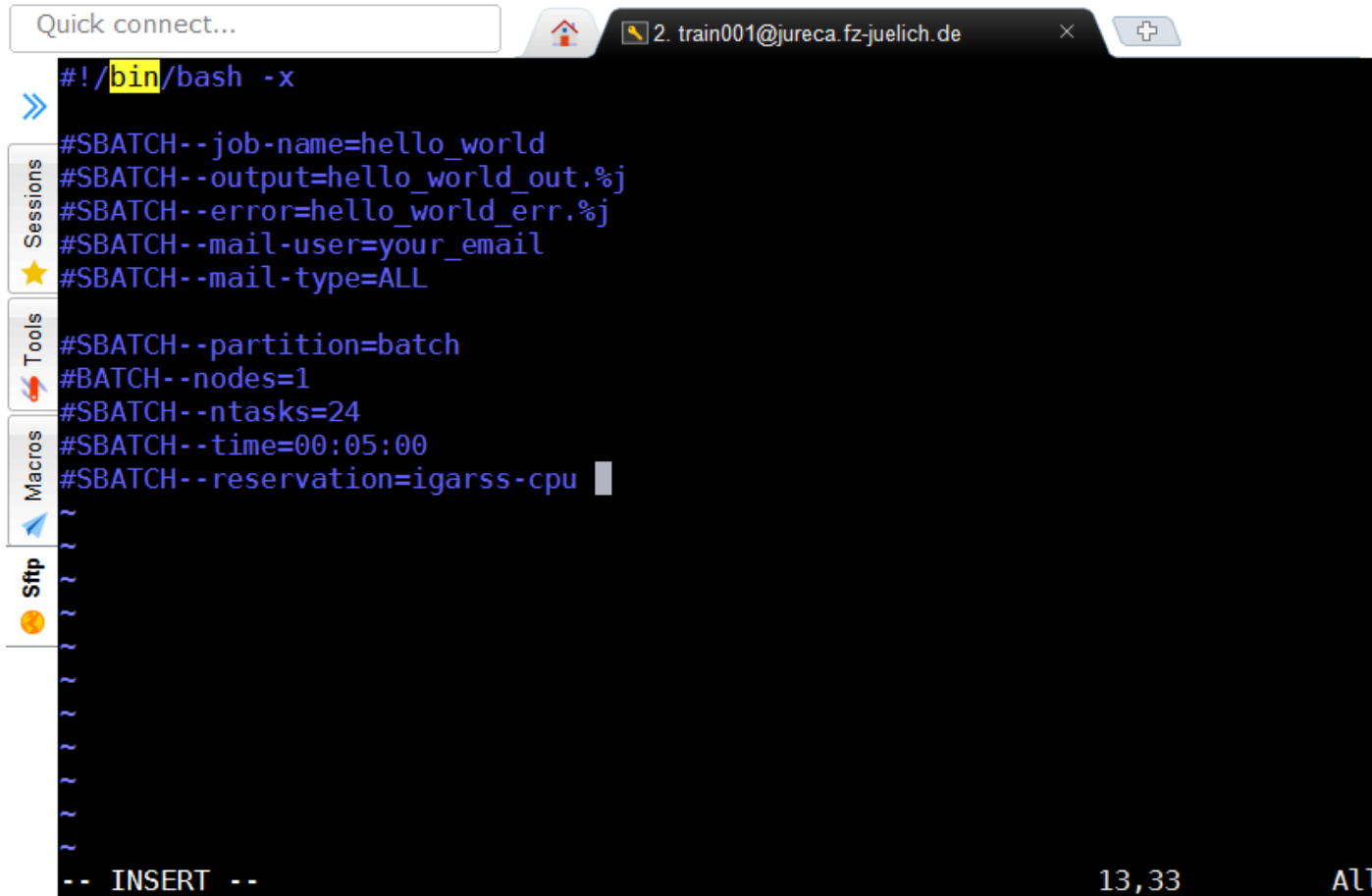


```
Quick connect... 2. train001@jureca.fz-juelich.de x +
#!/bin/bash -x
#SBATCH--job-name=hello_world
#SBATCH--output=hello_world_out.%j
#SBATCH--error=hello_world_err.%j
#SBATCH--mail-user=your_email
#SBATCH--mail-type=ALL
```

-- INSERT -- 7,24 All

- **#SBATCH--job-name=hello\_world**
  - Set the name of the job
- **#SBATCH--output=hello\_world\_out.%j**
  - Path to the job's standard output
- **#SBATCH--error=hello\_world\_err.%j**
  - Path to the job's standard error
- **#SBATCH--mail-user=your\_email**
  - Define the mail address for notifications
- **#SBATCH--mail-type=ALL**
  - When to send mail notifications  
Options: BEGIN,END,FAIL,ALL

# Job Scrip Editing (3)

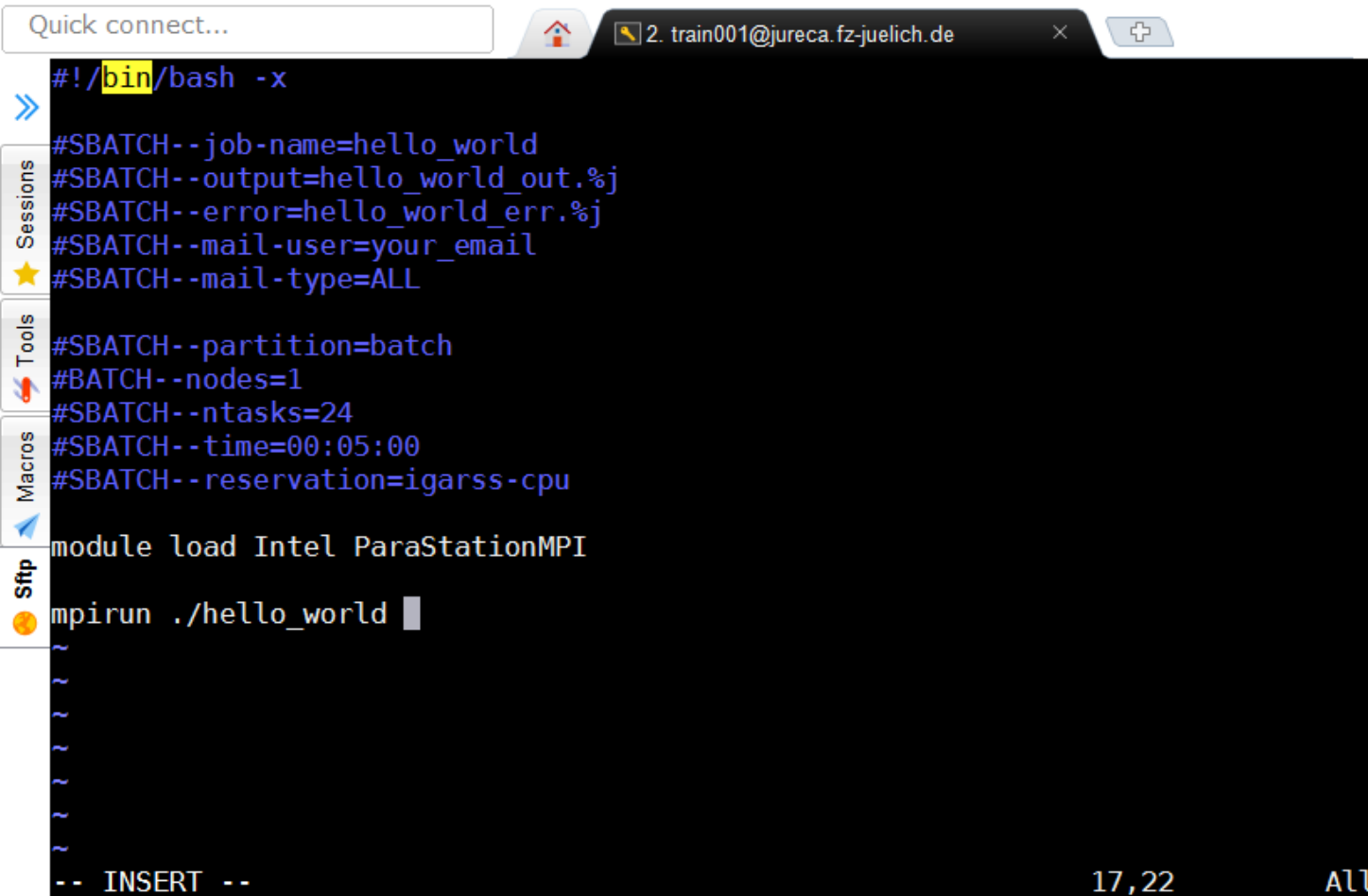


```
Quick connect... 2. train001@jureca.fz-juelich.de
#!/bin/bash -x
#SBATCH--job-name=hello_world
#SBATCH--output=hello_world_out.%j
#SBATCH--error=hello_world_err.%j
#SBATCH--mail-user=your_email
#SBATCH--mail-type=ALL
#SBATCH--partition=batch
#SBATCH--nodes=1
#SBATCH--ntasks=24
#SBATCH--time=00:05:00
#SBATCH--reservation=igarss-cpu
-- INSERT --
```

- **#SBATCH--partition=batch**
  - Partition to be used from the job
- **#SBATCH--nodes=1**
  - Number of compute nodes used by the job
- **#SBATCH--ntasks=24**
  - Number of tasks (MPI processes)
- **#SBATCH--time=00:05:00**
  - Maximum wall-clock time of the job
- **#SBATCH--reservation=igarss-cpu**
  - Use nodes reserved for this tutorial

(ReservationName=igarss-cpu StartTime=2018-07-22T10:45:00 EndTime=2018-07-22T18:15:00)

# Job Scrip Editing (4)

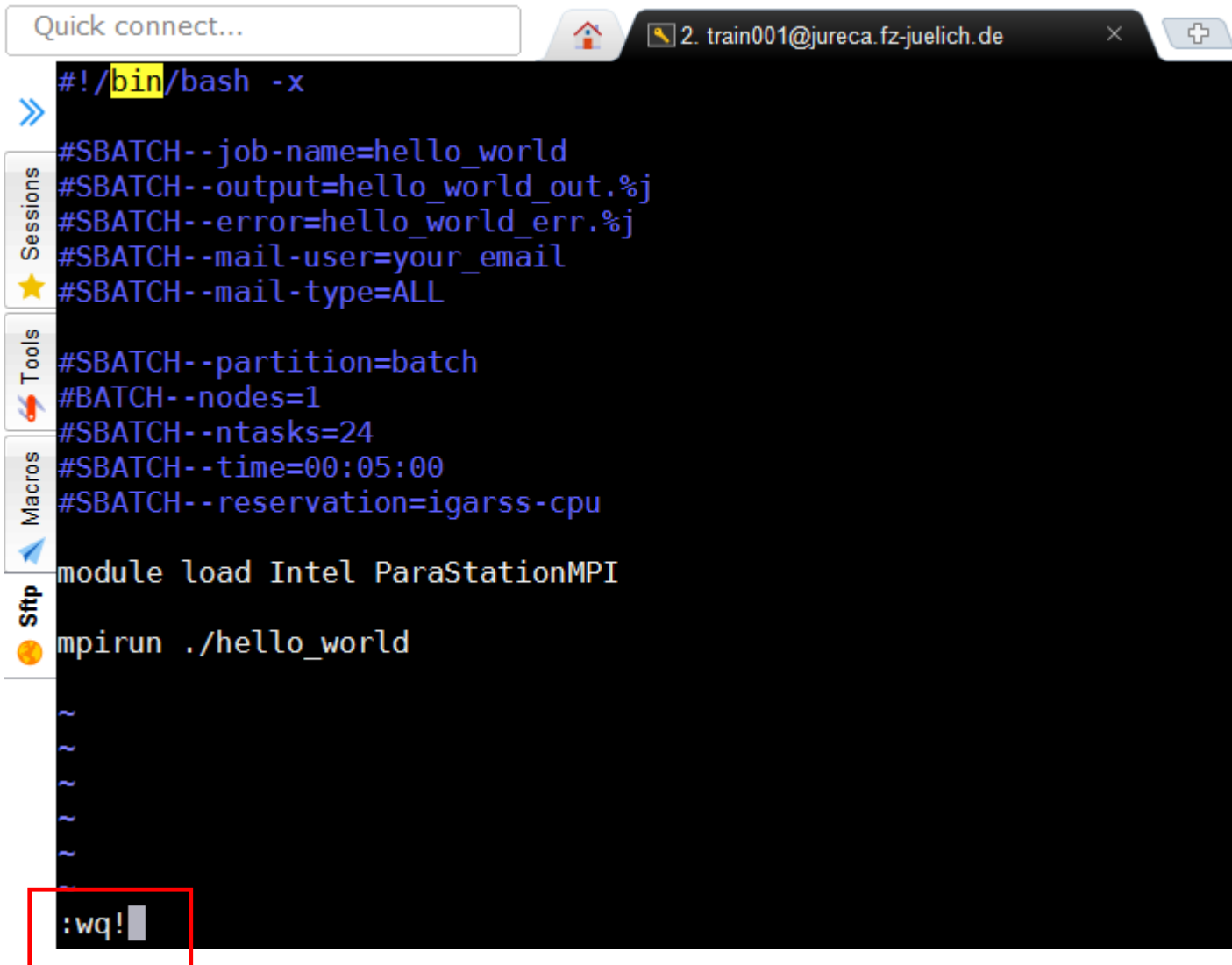


```
Quick connect... 2. train001@jureca.fz-juelich.de
#!/bin/bash -x
#SBATCH--job-name=hello_world
#SBATCH--output=hello_world_out.%j
#SBATCH--error=hello_world_err.%j
#SBATCH--mail-user=your_email
#SBATCH--mail-type=ALL
#SBATCH--partition=batch
#SBATCH--nodes=1
#SBATCH--ntasks=24
#SBATCH--time=00:05:00
#SBATCH--reservation=igarss-cpu
module load Intel ParaStationMPI
mpirun ./hello_world
```

-- INSERT -- 17,22 All

- **module load Intel ParaStationMPI**
  - Get access to a specific set of software and its dependencies
- **mpirun ./hello\_world**
  - Execute the MPI program

# Save and Close the Job Script



```
Quick connect... 2. train001@jureca.fz-juelich.de
#!/bin/bash -x
#SBATCH--job-name=hello_world
#SBATCH--output=hello_world_out.%j
#SBATCH--error=hello_world_err.%j
#SBATCH--mail-user=your_email
#SBATCH--mail-type=ALL
#SBATCH--partition=batch
#BATCH--nodes=1
#SBATCH--ntasks=24
#SBATCH--time=00:05:00
#SBATCH--reservation=igarss-cpu
module load Intel ParaStationMPI
mpirun ./hello_world
~
~
~
~
~
:wq!
```

- Press in this exact order the following keys of your keyboard:
- **ESC**
- **:**
- **w**
- **q**
- **!**
- **ENTER**

# Submit the Job Script

- **\$ sbatch submit\_hello\_world.sh**

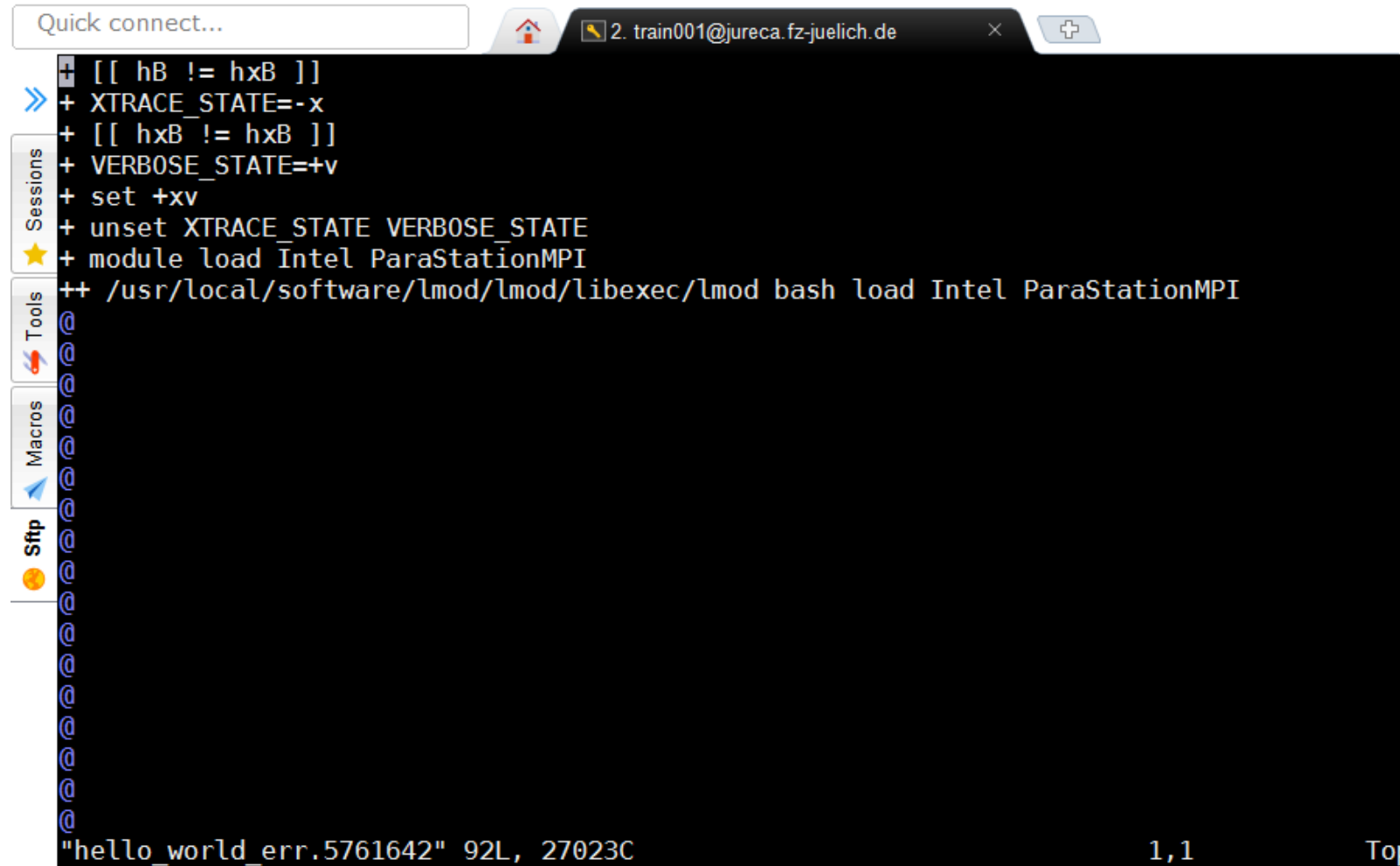
```
hello_world hello_world.c run_hello_world.sh
[train001@jrl10 mpi_hello_world]$ sbatch run_hello_world.sh
Submitted batch job 5761642
[train001@jrl10 mpi_hello_world]$ █
```

# Check the Results

- If the job was successfully run, you will get 2 files

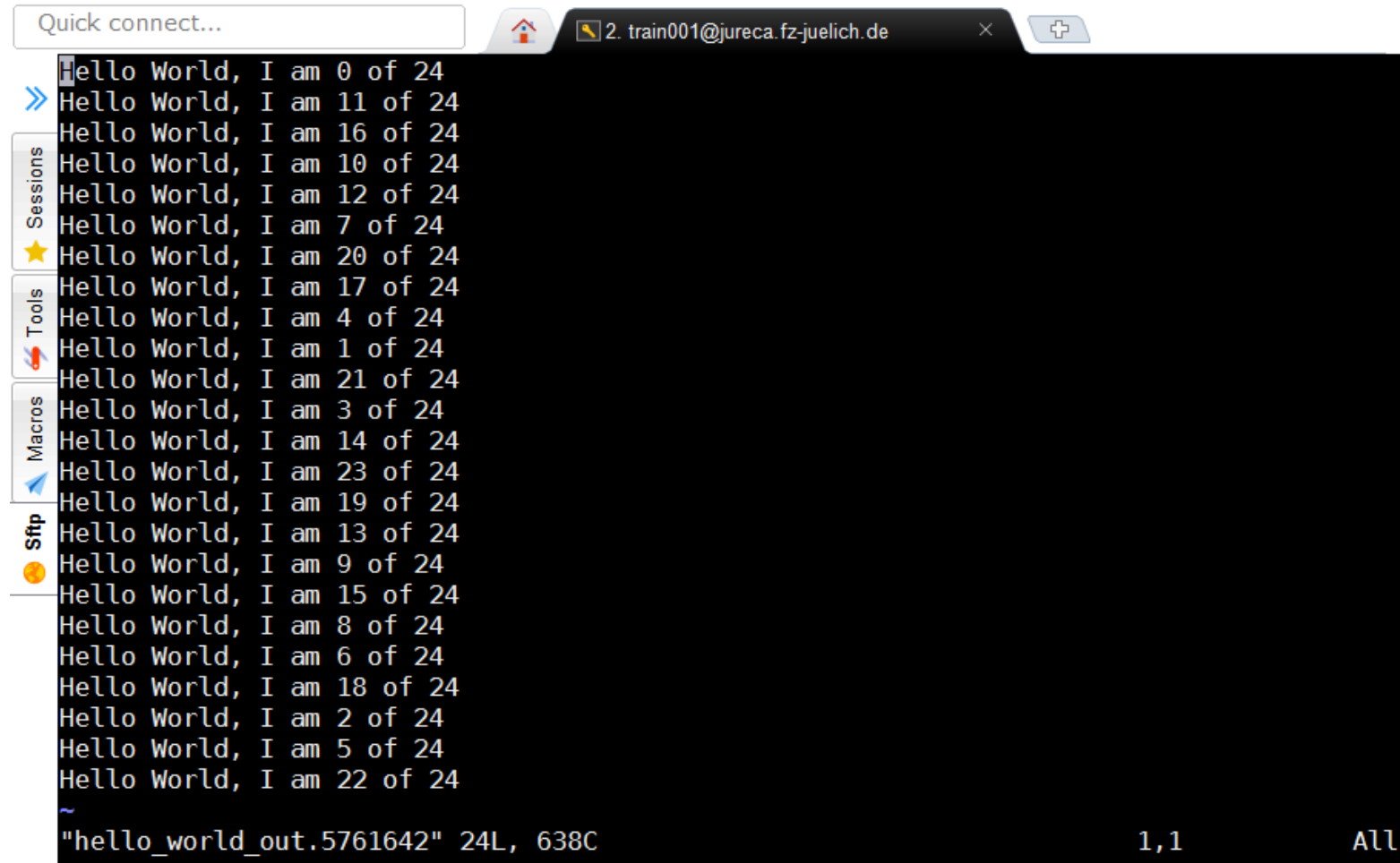
```
[train001@jrl10 mpi_hello_world]$ ls
hello_world hello_world_err.5761642 run_hello_world.sh
hello_world.c hello_world_out.5761642
[train001@jrl10 mpi_hello_world]$ █
```

# hello\_world\_err



```
Quick connect... 2. train001@jureca.fz-juelich.de
+ [[hB != hxB]]
+ XTRACE_STATE=-x
+ [[hxB != hxB]]
+ VERBOSE_STATE=+v
+ set +xv
+ unset XTRACE_STATE VERBOSE_STATE
+ module load Intel ParaStationMPI
++ /usr/local/software/lmod/lmod/libexec/lmod bash load Intel ParaStationMPI
"hello_world_err.5761642" 92L, 27023C 1,1 Top
```

# hello\_world\_out



```
Quick connect...
2. train001@jureca.fz-juelich.de
Hello World, I am 0 of 24
Hello World, I am 11 of 24
Hello World, I am 16 of 24
Hello World, I am 10 of 24
Hello World, I am 12 of 24
Hello World, I am 7 of 24
Hello World, I am 20 of 24
Hello World, I am 17 of 24
Hello World, I am 4 of 24
Hello World, I am 1 of 24
Hello World, I am 21 of 24
Hello World, I am 3 of 24
Hello World, I am 14 of 24
Hello World, I am 23 of 24
Hello World, I am 19 of 24
Hello World, I am 13 of 24
Hello World, I am 9 of 24
Hello World, I am 15 of 24
Hello World, I am 8 of 24
Hello World, I am 6 of 24
Hello World, I am 18 of 24
Hello World, I am 2 of 24
Hello World, I am 5 of 24
Hello World, I am 22 of 24
~
"hello_world_out.5761642" 24L, 638C 1,1 All
```

# Additional Material

# JURECA Partitions

| Partition                                 | Nodes         | Resources                                            | Walltime                          | MaxNodes  | Description                                                                                              |
|-------------------------------------------|---------------|------------------------------------------------------|-----------------------------------|-----------|----------------------------------------------------------------------------------------------------------|
| <i>batch</i>                              | 1712          | 24(48) CPU Cores<br>128/256 GB RAM                   | Default: 1 hour<br>Max.: 24 hours | 256       | Default partition, normal compute nodes (some with 256GB RAM)                                            |
| <i>devel</i>                              | 20            | 24(48) CPU Cores<br>128 GB RAM                       | Default: 30 mins<br>Max.: 2 hours | 8         | Partition mainly for develop-ment (interactive jobs)                                                     |
| <i>large</i>                              | 1712          | 24(48) CPU Cores<br>128/256 GB RAM                   | Default: 1 hour<br>Max.: 24 hours | UNLIMITED | Same as batch targeting big jobs (currently down)                                                        |
| <i>mem256</i>                             | 128           | 24(48) CPU Cores<br>256 GB RAM                       | Default: 1 hour<br>Max.: 24 hours | 128       | Fat compute nodes with 256GB RAM (also in batch)                                                         |
| <i>mem512</i>                             | 64            | 24(48) CPU Cores<br>512 GB RAM                       | Default: 1 hour<br>Max.: 24 hours | 32        | Fat compute nodes with 512GB RAM                                                                         |
| <i>mem1024</i>                            | 2             | 24(48) CPU Cores<br>1 TB RAM                         | Default: 1 hour<br>Max.: 24 hours | 2         | Fat compute nodes with 1TB RAM                                                                           |
| <i>gpus</i>                               | 70            | 24(48) CPU Cores<br>128 GB RAM<br>2x Nvidia K80      | Default: 1 hour<br>Max.: 24 hours | 32        | Compute nodes with 4 GPUs available (CUDA apps) (4 GPUs visible)                                         |
| <i>develgpus</i>                          | 5             | 24(48) CPU Cores<br>128 GB RAM<br>2x Nvidia K80      | Default: 30 mins<br>Max.: 2 hours | 2         | Partition for testing and development on the GPUs                                                        |
| <i>vis</i>                                | 10            | 24(48) CPU Cores<br>512/1024 GB RAM<br>2x Nvidia K40 | Default: 1 hour<br>Max.: 24 hours | 4         | Compute nodes with 2 GPUs, mainly for visualization SW                                                   |
| <i>booster</i><br>( <i>develbooster</i> ) | 1640<br>(32?) | 68 (272) CPU Cores<br>96/112 GB RAM                  | Default: 1 hour<br>Max.: 24 hours | 512       | KNL (Intel Xeon Phi) compute nodes with 96 or 112 GB memory (depends on config. of local memory of 16GB) |

[10] JURECA HPC System

\* Other partitions: *largegpus*, *largevis* (same as *gpus* and *vis* but with no max. nodes limit)

# System Usage – Modules

- The installed software of the clusters is organized through a hierarchy of modules.
- Loading a module adapts your environment variables to give you access to a specific set of software and its dependencies.
- Preparing the module environment includes different steps:
  1. [Optional] Choose SW architecture: Architecture/Haswell (default) or Architecture/KNL
  2. Load a compiler
  3. [Optional] Load an MPI runtime.
  4. Load other modules, that where built with currently loaded modules (compiler, MPI, other libraries)
- Useful commands:

|                           |                                           |
|---------------------------|-------------------------------------------|
| List available modules    | \$ module avail                           |
| Choose the SW Arch.       | \$ module load Architecture/[Haswell KNL] |
| Load compiler and MPI     | \$ module load Intel ParaStationMPI       |
| List all loaded modules   | \$ module list                            |
| List available modules    | \$ module avail                           |
| Check a package           | \$ module spider GROMACS                  |
| Load a module             | \$ module load GROMACS/<version>          |
| Unload a module           | \$ module unload GROMACS/<version>        |
| Unload all loaded modules | \$ module purge                           |

[10] JURECA HPC System

# Slurm – User Commands (1)

- **salloc** to request interactive jobs/allocations
- **sattach** to attach standard input, output, and error plus signal capabilities to a currently running job or job step
- **sbatch** to submit a batch script (which can be a bash, Perl or Python script)
- **scancel** to cancel a pending or running job or job step
- **sbcast** to transfer a file to all nodes allocated for a job
- **sgather** to transfer a file from all allocated nodes to the currently active job. This command can be used only inside a job script
- **scontrol** provides also some functionality for the users to manage jobs or query and get some information about the system configuration
- **sinfo** to retrieve information about the partitions, reservations and node states
- **smap** graphically shows the state of the partitions and nodes using a curses interface. We recommend **llview** as an alternative which is supported on all JSC machines

[12] SLURM Workload Manager



# Slurm – User Commands (2)

- **sprio** can be used to query job priorities
- **squeue** to query the list of pending and running jobs
- **srn** to initiate *job-steps* mainly within a job or start an interactive jobs. A job can contain multiple job steps executing sequentially or in parallel on independent or shared nodes within the job's node allocation
- **sshare** to retrieve fair-share information for each user
- **sstat** to query status information about a running job
- **sview** is a graphical user interface to get state information for jobs, partitions, and nodes
- **sacct** to retrieve accounting information about jobs and job steps in Slurm's database
- **sacctmgr** allows also the users to query some information about their accounts and other accounting information in Slurm's database.

\* For more detailed info please check the online documentation and the man pages

[12] SLURM Workload Manager



# Slurm – Job Submission

- There are 2 commands for job allocation: **sbatch** is used for batch jobs and **salloc** is used to allocate resource for interactive jobs. The format of these commands:
  - `sbatch [options] jobscript [args...]`
  - `salloc [options] [<command> [command args]]`
- List of the most important submission/allocation options:

|                                 |                                                              |
|---------------------------------|--------------------------------------------------------------|
| <code>-A --account</code>       | Charge CPU-Quota to specified account (budget ID).           |
| <code>-c --cpus-per-task</code> | Number of logical CPUs (hardware threads) per task.          |
| <code>-e --error</code>         | Path to the job's standard error.                            |
| <code>-i --input</code>         | Connect the jobscript's standard input directly to a file.   |
| <code>-J --job-name</code>      | Set the name of the job.                                     |
| <code>--mail-user</code>        | Define the mail address for notifications.                   |
| <code>--mail-type</code>        | When to send mail notifications. Options: BEGIN,END,FAIL,ALL |
| <code>-N --nodes</code>         | Number of compute nodes used by the job.                     |
| <code>-n --ntasks</code>        | Number of tasks (MPI processes).                             |
| <code>--ntasks-per-node</code>  | Number of tasks per compute node.                            |
| <code>-o --output</code>        | Path to the job's standard output.                           |
| <code>-p --partition</code>     | Partition to be used from the job.                           |
| <code>-t --time</code>          | Maximum wall-clock time of the job.                          |
| <code>--gres</code>             | Request nodes with specific Generic Resources.               |

*[12] SLURM Workload Manager*

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# **DEEP** *Projects*



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